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Comparative Application Of The EKMA In The Los Angeles Area

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The ability of seven models, ranging in sophistication from the SAI Urban Airshed Photochemical Grid Model to a published set of ozone isopleth curves (i.e., "standard" or Level IV EKMA) to predict peak ozone is examined for three days observing high ozone in the Los Angeles Basin. The impact of control strategies simulated with each of the models is also compared. Impact of specific differences among models such as different means of considering horizontal and vertical diffusion and use of different chemical mechanisms is also examined.

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EXECUTIVE SUMMARY

The Office of Air Quality Planning and Standards (OAQPS) of the U.S. Environmental Protection Agency (EPA) has for some time been examining the attractiveness of using grid-based, complex atmospheric simulation models for predicting and estimating reactive-pollutant concentration patterns that might result if a specific emissions control strategy were adopted in a particular urban area. Because of the complexity and the cost of such models, less complex models like EKMA are also being considered by several states for widespread applications in regulatory programs. As part of a major program, OAQPS is sponsoring a study of the use of complex grid models as a means for evaluating the simpler, less resource-intensive models. The study investigates three major approaches: (1) simplification of input information to existing complex models; (2) direct comparison of simple and complex model performance; and (3) use of complex models in a limited number of prototype cities representing a variety of meteorological/air quality/emissions combinations.

The primary objective of the study presented in this report is to compare the performance of the simple models with that of the more complex models.

The input files for the SAI Urban Airshed Model for three meteorological days were used to provide data for a comparison study of a series of trajactory models. Emission files projected for the year 1982 were also available so that comparisons between models could be made in order to project emission changes. The model series was developed to provide a basis of analysis in which the simplest model (the standard EKMA) could be compared to the most complex (the SAI Urban Airshed Model). The major findings of this trajectory model comparison study are organized according to the model series as follows:

> Although the SAI grid and SAI trajectory models share many algorithms in common, the two models may produce quite different results from the same input data. Along any given trajectory path the only major differences between the models are found in the grid model's ability to simulate wind shear, convergence, and divergence. However, the observations often agree more closely with

the simulations of the trajectory model than with those of the grid model. Hence, the wind fields used in the grid model may require some reevaluation. Comparisons for regions in which simple wind patterns are expected are being carried out in St. Louis and Tulsa. It is also recommended that trajectory model simulations be used to supplement grid-model simulations in general, especially for trajectories to the maximum observed or simulated ozone sites.

> The EKMA-type model with Carbon-Bond chemistry (CBM-EKMA) produced simulations of ozone levels fairly close to the levels simulated by the SAI trajectory model. Differences in the time dependence of ozone development for the two models suggest that the variable temperature used in the SAI trajectory model, when compared with the fixed temperature used in the CBM-EKMA, may cause the most significant difference in the results between the two.

> Comparisons of the CBM chemistry and the propylene/butane chemistry used in the regular EKMA model show that major differences can occur under certain circumstances. These differences apparently stem from reaction rate constant difference and from the balanced spectrum of species treated in the CBM compared with the polarized reactivity of propylene and butane. The differences appear to be a function of HC/NO_x concentration, and the two mechanisms lead to different control-strategy implications. Therefore, further study is required.

> Changes in propylene percentage or photolysis did not lead to significant differences in maximum ozone levels when the propylene/butane chemistry was used for this set of trajectories.

> Results using linear changes in mixing heights were compared with results from the city-specific EKMA, which uses only two mixing heights interpolated with an exponential function. The mixing-height changes found in the input files used for this particular study were, in general, adequately interpolated by the exponential function used in the EKMA.

> The city-specific EKMA trajectory results often agree with, or come close to, points on the standard EKMA isopleth by virtue of large compensating differences in

the models. Treatment of continuous emissions in the city-specific model tended to generate more ozone; however, large changes in mixing height tended to generate less ozone in the city-specific model than in the standard EKMA isopleth, which neglects continuous emissions and assumes a small change in mixing height.

Isopleth predictions by all the models tended to reflect the trajectory model results except when assumptions necessary to generate the diagrams differed from assumptions made in the SAI grid and trajectory model simulations.

A new type of isopleth diagram has been introduced during this study. The new diagram is based on emissions that use early trajectory-model starting times in order to minimize dependence on initial conditions. Further comparison of the two types of isopleths is necessary, but the findings of this study suggest that the new method predicts changes in ozone levels that are more consistent with changes in emissions than did the original isopleth approach.

I THE MODEL SERIES

The various applications of the SAI Urban Airshed Model to the Los Angeles area provide a special opportunity for a comparison of the results of those applications with the results of other models, particularly with those of the SAI trajectory model and with versions of the trajectory model used in the EKMA. If we arrange these models in a series on the basis of model complexity,* with a high degree of commonality among the models, comparisons of results between adjacent models can be made in a way that minimizes the number of model differences involved.

A similarity in the results of adjacent models would indicate that for the particular case studied the differences in complexity were not important. Correspondingly, a large difference in results would apparently indicate that the features uniquely addressed by the more complex model were significant for that case.

This section describes such a model series and comparison study using six Airshed Model runs. Only three meteorological days were used for the study: 26 June 1974, 27 June 1974, and 4 August 1975. The SAI Airshed Model was run for each meteorological day, using emissions files for the 1975 base year and projected emissions for 1982.

The following list briefly describes the series of seven models used in this study. More detailed descriptions of the models are given as each model comparison is discussed. Some models are distinguished only by the mode of application.

1) The SAI Urban Airshed Model.

2) The SAI trajectory model (the only difference between this model and 1)--in terms of inputs, computations, and results at points along a selected trajectory--is the elimination of horizontal dispersion and convergent and divergent winds).

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* By model complexity we mean the spatial and temporal detail with which the modeling is executed and also the detail with which the physical and chemical processes are represented.

3) An EKMA-style model (CBM-EKMA), with the same chemistry (carbon bond) and mixing heights as the SAI trajectory model (in this case the main differences are in the use of fixed concentrations aloft, elimination of eddy diffusion, and the use of a Gear-type integration scheme instead of a steady-state scheme with finite differencing).

4) The same EKMA-style model (EKMA IIa), with the standard propylene/butane chemistry but with modified photolysis rates.

5) The same EKMA-style model (EKMA IIb) with standard photolysis rates.

6) The same EKMA-style model (EKMA IIc), with constant dilution determined from two mixing heights (i.e., the regular city-specific OZIPP model).

7) The "standard" Los Angeles EKMA.

II MODEL COMPARISONS

A. COMPARISON OF SAI GRID AND TRAJECTORY MODELS*

The model series begins with the SAI grid model and ends with the "standard" Los Angeles EKMA trajectory model. The first "step" in the series is from the SAI grid to the trajectory model. This step involves a major transition for the entire series from the grid concept to the moving air parcel trajectory concept. Therefore, we must carefully compare the differences and similarities between these two SAI models.

The two models were designed to complement each other and many algorithms are identical for both models (several subroutines of the computer codes are actually shared); furthermore, both models use the same input files. The trajectory model begins on a square of the grid model at a specific time. The path of the trajectory is then determined solely by the wind speed and direction in the lowest level of the grid-model files. Because the other levels in the grid model often advect with velocities that are different from this lowest level, the two models often generate different results as the simulations progress in time. Nevertheless, the trajectory model provides an inexpensive method for testing parts of the grid model.

A special feature of the SAI trajectory model is that it can be operated backward in time. This feature was used to generate the trajectories used in this study. The time and location of either the observed (for the base-case days) or the simulated (for the 1982 days) ozone maximum were used to start the backward trajectory to 0400 hours. Thus the forward trajectories always arrived at the desired spot at the proper time for comparison with either observations or grid-model results. A major shortcoming inherent in the use of any trajectory model as a tool for control strategies is that changes in emissions often lead to changes in the time and location of maximum ozone concentrations. Small changes in times of maximum ozone concentration at some specific monitoring site can be associated with rather large differences in the origin of the trajectory

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* Detailed discussions of this comparison are available elsewhere (see Reynolds et al., 1979).

paths. Because the trajectory model is fixed to a specific path, it would overestimate the effectiveness of emission controls at the monitoring site if used for control-strategy estimates.

B. COMPARISON OF THE SAI TRAJECTORY MODEL AND THE CBM-EKMA MODEL

The step in the model series from the SAI trajectory model to the model we call the CBM-EKMA represents the first step into the generic set of EKMA-type models; all these models can be run with the computer program known as OZIPM. Therefore, comparisons of the SAI trajectory model and the EKMA-type model, which is as similar in design as is possible without major changes in computer coding, are particularly significant.

The following similarities and differences exist between the SAI trajectory model and the EKMA developed for this comparison:

- Chemistry--Both models use a carbon-bond chemistry that is also identical to the chemistry currently used in the SAI grid model. However, the photolytic constants are computed differently in the EKMA and SAI models. For this study, we modified the regular EKMA values for NO_2 photolysis using a constant factor so that all models agreed at 1300 PDT. In the Airshed Model and trajectory model, all other photolysis rates vary with NO_2 photolysis, with a fixed ratio for each; but in the EKMA, the photolysis rates vary independently. Aldehyde photolysis was adjusted in the EKMA to give agreement between the models at 1100 PDT.

  Actually, these differences in photolysis rates constitute an advantage in sophistication for the EKMA. The NO_2 photolysis rates normally used in the EKMA are somewhat lower than those used in the SAI models because the latter formerly used an algorithm based on older data. Incidentally, the SAI models are now being updated to the EKMA NO_2 photolysis rates, which are those recommended by Demerjian, Schere, and Peterson (1980). Since the purpose of the present study was to compare the EKMA with previously computed results of the Airshed Model, we were forced to alter the EKMA models to eliminate this difference, rather than wait for the older SAI studies to be rerun with the newer photolysis rates for NO_2.

  The improved treatment of aldehyde photolysis rates in the EKMA over that of the Airshed Model is similar to use of

the numerical scheme of Gear rather than the steady-state/Crank-Nicholson method. Such improvements would be too costly for the SAI model. The use of fixed ratios of NO_2 photolysis in the SAI models in place of the variable ratios used in the EKMA model may lead to some minor differences in chemistry. The ratios are at a maximum at solar noon and a minimum at sunrise and sunset (Whitten, Killus, and Hogo, 1980). The photolysis rates for aldehydes change more with solar zenith angle than the NO_2 photolysis rate does because aldehydes photolyze at the short wavelength end of the solar spectrum, whereas NO_2 photolyzes nearer the long wavelength end of the ultraviolet spectrum. The short ultraviolet wavelengths are more affected by the ozone in the stratosphere than are the longer wavelengths. At high zenith angles (morning and evening), the solar rays must pass through a thicker layer of ozone. Therefore, the ratio of aldehyde photolysis to NO_2 photolysis varies throughout the day, reaching a maximum at solar noon.

For this particular study, the EKMA aldehyde photolysis values were multiplied by a constant value throughout each day so that the models agreed at 1100 PDT. Therefore, in the early morning the photolysis rate of the aldehydes in the EKMA would be somewhat less than that used in the SAI models. This effect would add to the expected increase in reactivity in the mornings for the SAI models as a result of the steady-state approximations. Since the steady-state approximation assumes an instantaneous buildup of the steady-state species, the chemistry would be expected to proceed faster in the early morning for models using this approximation than for models of the EKMA type. These models do not use steady-state conditions and, in addition, the species build up gradually because of the slow photolysis rates that occur in the morning. However, the comparisons made in this study usually showed the opposite, namely, that the EKMA models were slightly more reactive in the mornings. The reasons for the occurrence of this anomaly are unknown at this time.

For this particular study, we chose to modify the CBM-EKMA to make it as much like the Airshed Model and trajectory model as possible. By removing all possible potential variables between models, we hoped to be able to better compare their underlying principles. For comparisons involving the regular EKMA, we chose to use that model in

the manner in which it might normally be applied. The CBM version of EKMA has normally been applied to assist users of the Airshed Model to estimate potential control scenarios. For such applications the photolysis adjustments discussed here are normal. Perhaps for this study an additional series of tests with CBM-EKMA using the regular EKMA photolysis rates would have been helpful, but they were not performed during that phase of the contract.

- Reactivity--The SAI Trajectory and Grid models are operated with reactivity splits that vary with each source category. However, the EKMA-type models do not have this feature; reactivity is assumed to be constant for all hydrocarbon emissions throughout the day. For this study the OZIPM computer code was modified so that three different hydrocarbon reactivities could be used: one for the initial conditions, one for the aged hydrocarbons aloft, and one for the emissions that occur throughout the day. Hence the only differences in reactivity were in the temporal variations aloft and in the variable emissions used in the SAI models compared with the fixed reactivities employed in the emissions for the EKMA models. The reactivities used in the CBM-EKMA were determined from averages of emissions used in the SAI trajectory model; for hydrocarbons aloft a weighting factor was used each hour that was equal to the positive change in mixing height.

  In a sense, the NO_2/NO_x ratio also acts as a reactivity effect. The EKMA-type models all use a fixed ratio of NO_2/NO_x (10 percent) for all NO_x emissions, whereas the SAI models allow this ratio to vary according to their source category (the average ratio is typically about 5 percent). At this time, we have not attempted either to change the EKMA or to fix the ratio in the SAI model, because we feel the difference is trivial. For NO_x aloft, the EKMA uses pure NO_2, which is close to typical values found in the SAI trajectory model simulations; the calculated NO_2/NO_x ratio is almost always greater than 0.85, often with values greater than 0.99.

- Integration Scheme--The EKMA uses a Gear-type method without any steady-state approximations, whereas the SAI trajectory model uses the same Crank-Nicholson finite differencing scheme and steady-state approximations that are

used in the SAI grid model. Again, this difference in model sophistication is opposite to the direction intended by our series of models. However, our previous tests using smog chamber experiments suggest that the differences introduced by the numerical integration schemes should be minimal. Although the Gear integration scheme is well established for use in chemical kinetics calculations, the computer time and storage requirements are large. Use of more efficient schemes, such as the Crank-Nicholson technique employed in the SAI Airshed and trajectory models, requires the consideration of many species in steady state. In addition to reducing the requisite size of the system, the steady-state approximation helps eliminate a problem arising from stiffness. This mathematical property, common to most chemical kinetic systems, is a result of some parts of the system changing much more quickly than others.

Although the steady-state approximations for the CBM-have been carefully chosen and tested, there is no guarantee that the differences in results between the stiff-stable Gear method and the steady-state Crank-Nicholson method will be small compared with the other model differences studied here (such as eddy-diffusion and multiple vertical layers). Physically, the steady-state approximation implies that the mass of the steady-state species is insignificantly small and that these species are created and destroyed instantaneously. The first implication leads to mass balance problems when a species considered in steady state is large in concentration compared with its precursors or products. The second implication is most severely tested in atmospheric models during sunrise and sunset conditions when the photochemistry may be proceeding extremely slowly.

> Vertical Layers--The SAI grid and trajectory models share the same vertical layers and algorithms for numerical integration, but additional contributions are introduced into the grid model for convergent or divergent winds. The EKMA, of course, is limited to providing calculations of the mixed layer as a whole, but fixed concentrations in the layer aloft can be introduced as the mixing height rises. The SAI models account for mixing within the mixed layer, mixing within the inversion layer, and eddy diffusion among all layers. The EKMA assumes instantaneous mixing within the entire mixed layer, and no eddy diffu-

sion is considered across the boundary defined by the mixing height.

In our comparison studies, the effectiveness of multiple layers and eddy diffusion was one of the central issues to be evaluated by means of the models in this region of our model series. A problem that we tried to avoid, which does confound the comparison, is the entrainment of pollutants from aloft. The EKMA requires fixed concentrations aloft, so these must be chosen from some "proper" average of the time-dependent concentrations computed in the SAI trajectory model. With the average used in this study we attempted to weight most heavily the concentrations entrained when the mixing height rises most significantly. A more complex weighting scheme might involve the time when the greatest effect on the chemistry occurs; however, this effect was not evaluated. Concentrations aloft are not considered for the time before the inversion rises or after it has reached some maximum. As the mixing lid drops late in the afternoon, the only process affecting the surface layer from concentrations aloft is eddy diffusion. Eddy diffusion is treated in the SAI grid and trajectory models but is neglected in the EKMA.

> Mixing height--All models used in the EKMA that are based on the OZIPM computer code, as well as the SAI grid and trajectory models, can use identical mixing heights with values that vary linearly in time between specified values at each hour. However, the SAI models have a special arbitrary feature that can produce mixing-height profiles different from those of the EKMA. Minimum (50 m) and maximum (300 m) values for the heights are specified in the SAI models used in this study. When the mixing height is between 100 meters and 600 meters, the SAI models have two equal levels below the mixing height, and two equal levels between the mixing height and the top of the modeling region (1000 m). For all such cases the EKMA and the SAI models use mixing heights that vary with time in the same fashion. However, these two models may not have identical mixing heights for heights less than 100 m or more than 600 m. The SAI models linearly interpolate a value of mixing layer thickness called DIFBREAK at each time step from the mixing-depth input at each hour. However, below 100 meters and above 600 meters the size and the number of the cells with rapid mixing does not correspond to two equal cells below DIFBREAK. If DIFBREAK

falls below 52.5 meters the SAI models use one cell of 50 meters with rapid mixing. When the computed value of DIFBREAK goes above 52.5 meters, two cells of 50 meters each are suddenly treated with rapid mixing parameters. Above 600 meters, two cells of 300 meters each are used until the computed value of DIFBREAK reaches 630 meters, at which time a third cell of 200 meters is suddenly added, bringing the effective mixing height to 800 meters.

- Temperature--The temperature varies in the SAI grid and trajectory models, but the EKMA presently employs a fixed temperature. This difference can be significant. Temperature directly affects both vertical diffusion and chemistry in the SAI grid and trajectory models, but it can affect only chemistry in the EKMA models because vertical mixing is assumed to occur instantaneously within the mixed layer.

- Emissions--The SAI Airshed Model and trajectory model allow for emissions into all layers; the EKMA treats all emissions in the mixing layer alike and does not directly address emissions above the mixing layer. For the layer aloft in the EKMA, the emissions must be accounted for in the determination of the fixed concentrations aloft. The sum of the emissions used in the lower layers of the SAI trajectory model was used for the mixing layer in the EKMA.

  The EKMA was modified for this study to treat emissions in an absolute fashion rather than as a multiple of the initial conditions. This was implemented by treating the initial conditions as pollutants in the transported surface layer for the EKMA, but the normal initial condition (for the CALC mode in OZIPP or OZIPM) was specified as 1.0 for both HC and NO_x. The OZIPM computer code was modified slightly to ignore this specification of 1.0 as an initial condition. However, the multiplication of this number times the emissions was retained to allow the generations of isopleths on a scale relative to the base case emissions.

  Emissions for the SAI grid and trajectory models are given as total moles emitted into each cell during each hour. To arrive at values appropriate for the EKMA we used the following conversion procedure: The mixing volumes of the SAI trajectory model and the EKMA were assumed to be equal below the mixing height, such that

$$V = A \times Z_{mix} \quad ,$$

where A is the area and Z_{mix} is the mixing height. If the volume is expressed in cubic centimeters, the moles emitted in one hour (the number available from the trajectory model computer output) can be divided by this volume to give moles-cm^{-3} units. This, in turn, can be readily converted to the EKMA units of concentration, ppm, by using a conversion factor of 2.445×10^{10} ppm $moles^{-1}$ cm^3, which is technically correct for a perfect gas at 298 K and 1 atmosphere of pressure. The numbers calculated at this point are almost directly applicable to models used in the EKMA that are coded in both OZIPP and OZIPM. First, the use of 1.0 for the initial concentrations of HC and NO_x in the CALC mode implies that each one-hour emissions number would be the concentration added during the hour if the mixing height were the same as the initial value Z_0. However, the computer codes are written so that, at each instant in time, the emissions factor is multiplied by Z_0/Z_{mix}. Therefore, the Z_{mix} drops out and the actual numbers (En) used are merely

$$En = A \times 2.445 \times 10^{10}/Z_0 \quad ,$$

where A and Z_0 are in centimeter units.

In this particular study it was necessary to use special emission factors occasionally. These factors were used for those cases in which the SAI trajectory model employed substantial initial conditions for the first two layers (up to 100 m) even though the mixing height was only 50 meters. Since there was typically an order-of-magnitude difference in concentration between the initial conditions below 100 meters and the layers above this level, there was no way to compute a reasonable average to be used in the EKMA for the layer aloft. Hence the initial conditions used in the SAI models between 50 meters and 100 meters were treated as emissions in the EKMA models. These "emissions" were added to the normal emissions during the hour when the mixed layer in the SAI models jumped from 50 meters to 100 meters. For these cases the appropriate EKMA emissions factors merely add to the

normal emissions, since the initial mixing height is 50 meters and the height added is also 50 meters.

C. COMPARISON OF THE CBM-EKMA WITH A SIMILAR MODEL USING THE REGULAR EKMA PROPYLENE/BUTANE CHEMISTRY

The obvious intention of this comparison was to evaluate only the differences in the carbon-bond chemistry used by the SAI models and that used in the standard versions of the EKMA. Although the OZIPM computer program was specifically written to handle such comparisons, some complications were introduced when the EKMA was operated with the propylene/butane chemistry. First, the NO_2 and aldehyde photolysis rates were changed to make the carbon-bond and the propylene/butane mechanisms compatible. The NO_2 photolysis rates presented no problem since they were modified to be identical with the model using the CBM; this adjustment was discussed in the comparison of the SAI and CBM-EKMA models. For the aldeydes, it was assumed that the molecular concentrations of formaldehyde and acetaldehyde were always equal. The CBM used in this study assumes that the amounts of formaldehyde plus ketones is equal to the sum of the higher aldehydes. The aldehyde photolysis for the EKMA propylene/butane mechanism needed to be adjusted downward by a factor of three to ensure that the radical inputs for both mechanisms were equal at equal levels of total carbonyl concentration. Many studies, such as Whitten, Killus, and Hogo (1980), have shown that the input rate of radicals from aldehyde photolysis is about the most sensitive single factor in smog chemistry. We felt that a comparison of the CBM-EKMA and a model using the standard propylene/butane chemistry of EKMA would show the differences in the chemical mechanisms more clearly if the radical input rates were matched. However, we were concerned with the effects of these adjustments to the standard chemistry, so the next step in the model series involved only the reestablishment of the value of standard photolysis factors.

The reactivity of the two mechanisms was occasionally adjusted in this study. The total HC concentrations and emissions rates were identical for these two models, but the standard EKMA propylene/butane chemistry was typically used with the standard 25 percent propylene, 75 percent butane, and 5 percent aldehyde reactivity. When the two mechanisms did not produce similar results, attempts to match results were sometime made by varying the reactivity of the propylene/butane mix.

D. COMPARISON OF THE PROPYLENE/BUTANE EKMA MODELS USING ADJUSTED OR STANDARD PHOTOLYSIS RATES

As just discussed, the model closest in the model series to the CBM used specially adjusted NO_2 and aldehyde photolysis rates. For the individual trajectory-model runs, the comparison, at this point in the model series, illustrates the sensitivity to the photolysis constant adjustments. For the control-strategy assessment study using isopleth diagrams, we chose this point in the model series to convert from isopleths based on emissions inventories (the models were started at 0400) to isopleths based on 0800 initial precursor concentrations. The details of the isopleth construction and use are discussed later.

E. COMPARISONS OF THE REGULAR CITY-SPECIFIC EKMA MODEL AND THE SAME MODEL USING TIME-DEPENDENT MIXING-HEIGHT INPUT

The only difference between the EKMA just discussed, which uses the standard photolysis rates, and the regular city-specific EKMA regarding the OZIPP computer code is the use of variable mixing-height inputs in the former, more sophisticated version. In the propylene/butane version of the EKMA just discussed, instantaneous mixing heights are computed by linear interpolations between hourly input values rather than by the OZIPP method, which uses an exponential interpolation between the morning and afternoon mixing heights. The exponential increase in mixing height with time provides a constant dilution factor. In addition to the potential problems associated with the assumed shape of the mixing-height time profile, the standard EKMA cannot consider a decrease in mixing height that may follow an increase, nor can it consider a resumption in mixing-height growth following a decrease or a pause. However, the Los Angeles area has relatively less variance in mixing heights than other cities, so this aspect of the model series is not severely tested in this location.

F. COMPARISONS OF THE CITY-SPECIFIC EKMA AND THE STANDARD EKMA

This particular study involved the city of Los Angeles, which provided the basis for the standard EKMA. Hence the longitude and latitude used, as well as the time of year, are quite similar for these two modeling approaches. The main differences occur in mixing heights, materials aloft, and post-0800 emissions.

III COMPARISON OF MODEL RESULTS

The results of applying the seven models over the six trajectories are given in table III-1 and comparisons of certain results are illustrated in figure III-1. The paths of the six trajectories are illustrated in figures III-2 through III-7. In each case the trajectory was determined by running the SAI trajectory model backward with the chemistry turned off. For the three base-case days, the trajectories were determined so that the maximum observed ozone occurred in the trajectory model. For the 1982 days, the location of the predicted maximum ozone grid square in the SAI Urban Airshed Model was used to start the backward trajectory. Details of the input data are given in tables III-2 through III-10.

The early-morning start (0400) of the trajectory used in this study raises questions about uncertainties in wind patterns and mixing depths that can occur in the predawn hours. Therefore, the following information is given to help clarify the use of trajectory models such as the EKMA-type model in simulating the hours up to the normal starting time of 0800:

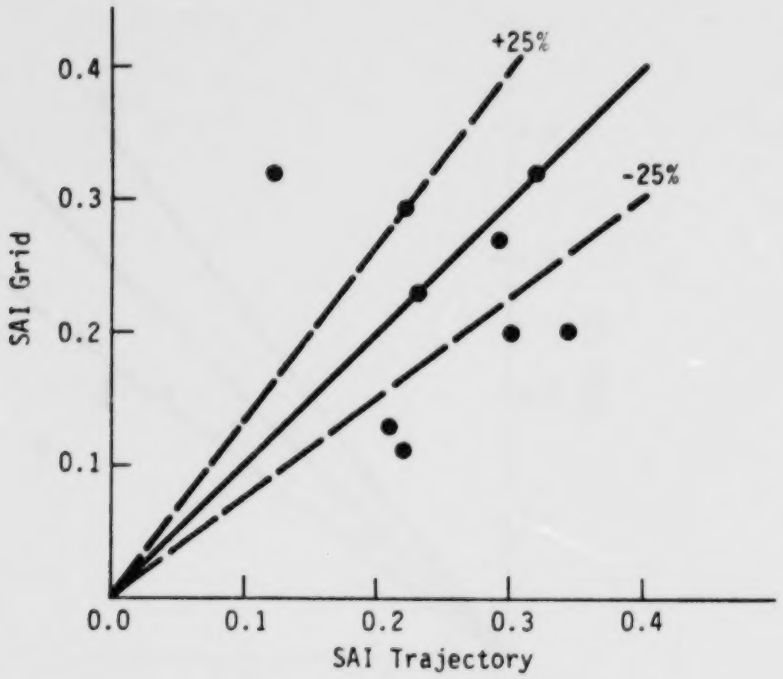
- Wind speeds in the early hours are not typically rapid so that the distance traveled up to 0800 would not be great. Hence the critical input data involved here, the emissions densities, should not be significantly affected by an ill-defined pathway. A general rule to consider would be the resolution and spatial variance of the emission inventory compared to the length and uncertainty of the early-morning pathway.

- Chemistry in the predawn hours is not sensitive to concentration, so the actual mixing heights used in the model up to 0800 are not critical (within some reasonable range). When the photochemistry becomes active around 0800, the mixing depth becomes more important, but this quantity is better defined. Since emissions are treated in an absolute fashion, the mixing heights used prior to 0800 would not affect the concentrations at 0800. Of course the initial conditions used at the start of the simulations (in the present case, 0400) would be affected

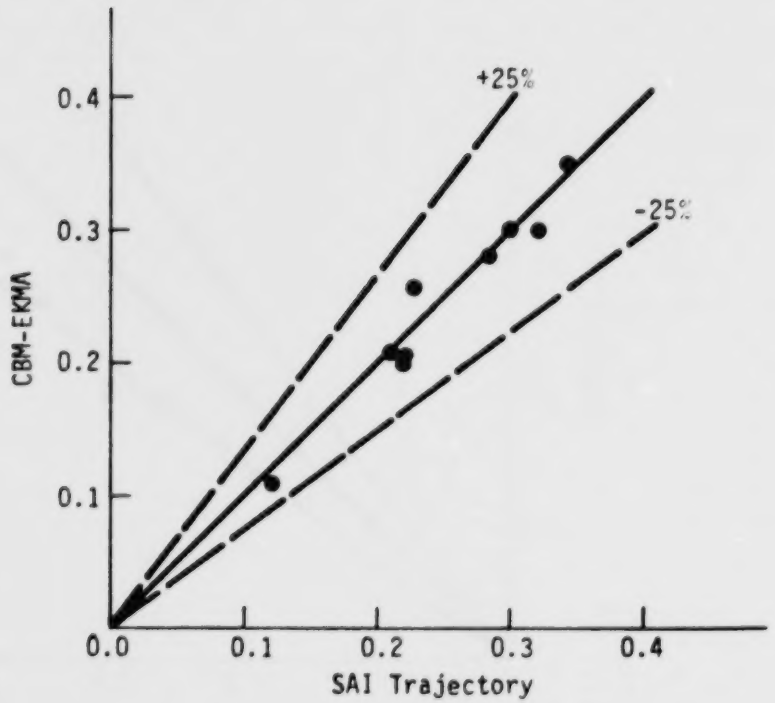
TABLE III-1. OZONE CONCENTRATION FOR NDI MODELING DAYS

Date	Location	Maximum Observed	SAI Airshed Predicted	SAI Trajectory Predicted	CBM-EKMA†	EKMA IIA†	EKMA IIB	City Specific Standard EKMA (Expotential Mixing Height	Standard EKMA	Time to Ozone Peak (PST)
26 June 1974	Fontana	0.34	0.20	0.30	0.30	0.19	0.20	0.20	0.16	1500
27 June 1974	Upland	0.49	0.32	0.32	0.30	0.21	0.21	0.22	0.30	1400
4 August 1975	Fontana	0.32	0.20	0.34	0.35	0.26	0.28	0.29	0.23	1300
26 June 1982	between Azusa/Upland		0.29	0.22	0.20	0.18	0.20	0.20	0.12	1500
27 June 1982	Upland		0.32	0.12	0.11	0.09	0.09	0.09	0.08	1600
4 August 1982	near Upland		0.23	0.23(0.10)§	0.26	0.20	0.19	0.21	0.12	1400
26 June 1982	Fontana*		0.13	0.21	0.208(0.195)§					1500
27 June 1982	Upland*		0.27	0.286	0.28					1400
4 August 1982	Fontana*		0.11	0.22	0.20					1300

* Same trajectory as the base case (74/75).
† Photolysis matched with SAI models.
§ Numbers in parenthesis explained in text.

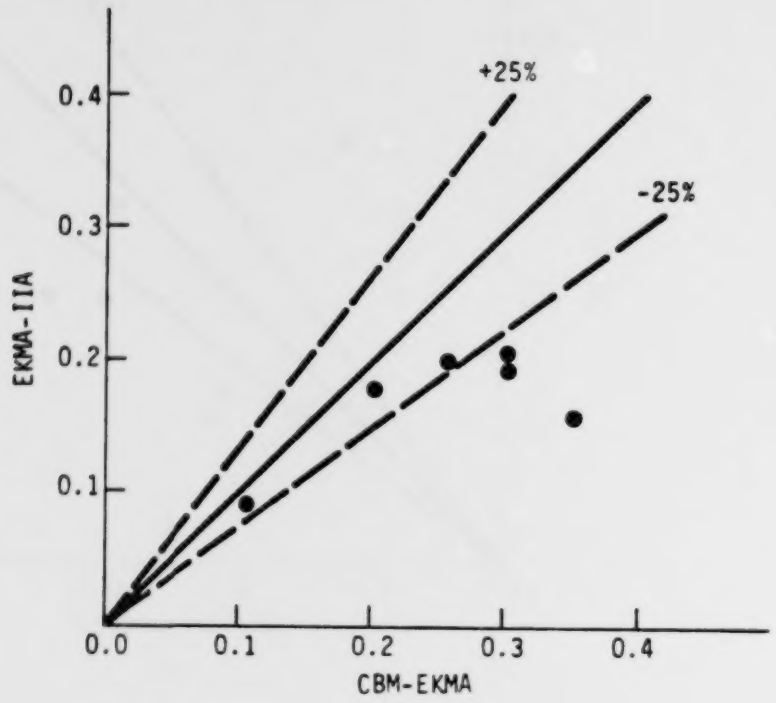


(a)

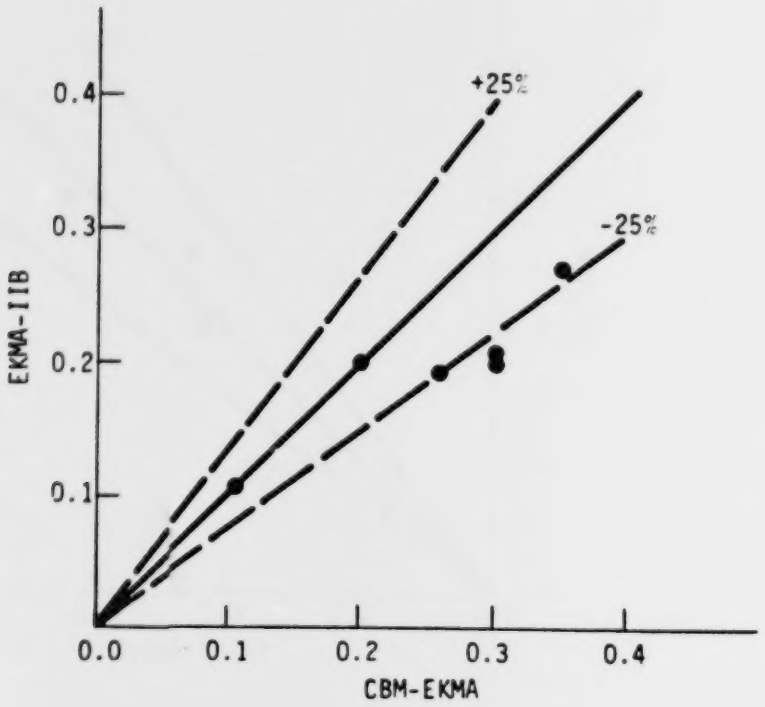


(b)

FIGURE III-1. SCHEMATIC COMPARISON OF MODEL RESULTS



(c)



(d)

FIGURE III-1 (Concluded)

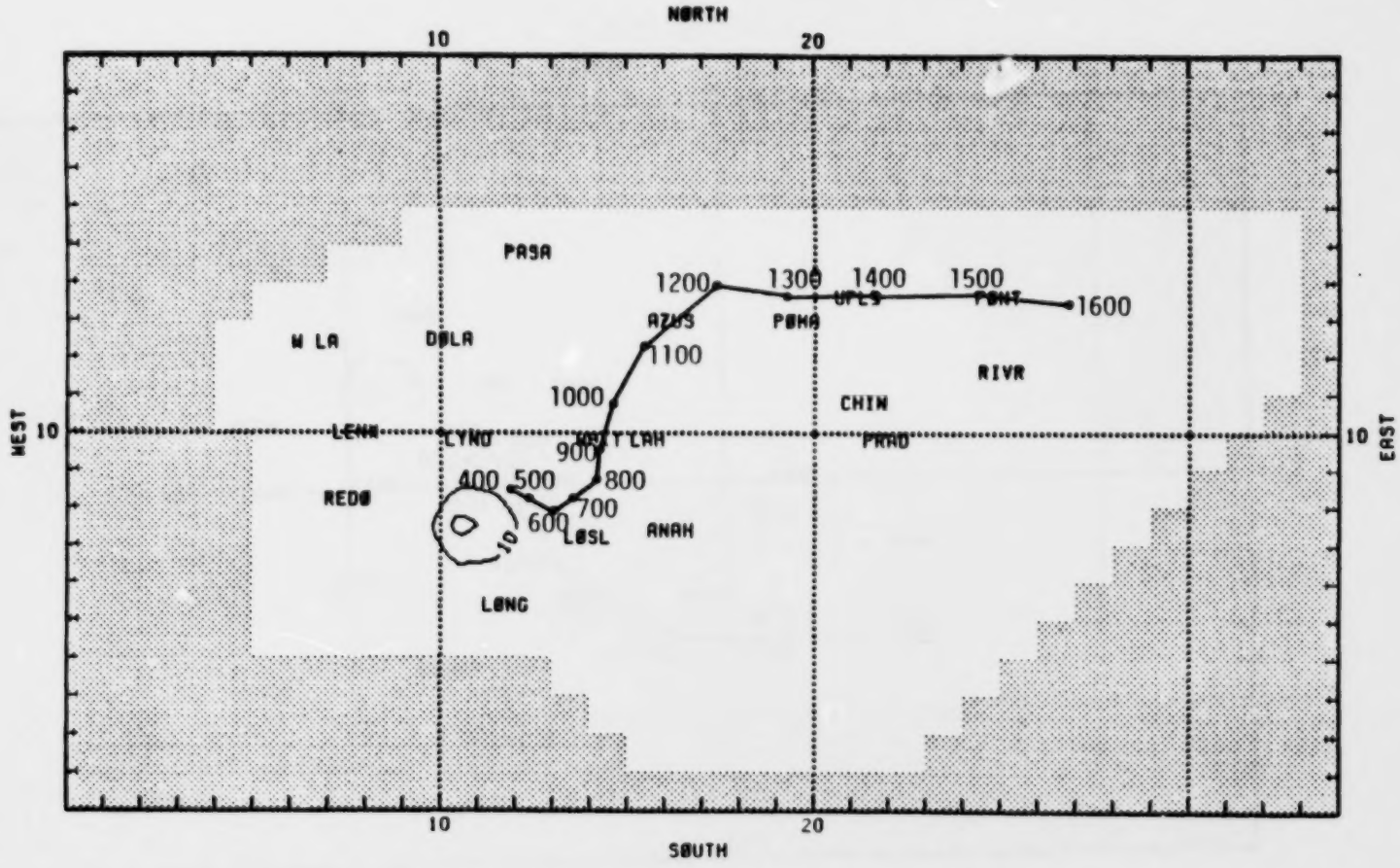


FIGURE III-2. TRAJECTORY USED FOR THE EKMA STUDY OF 26 JUNE 1974

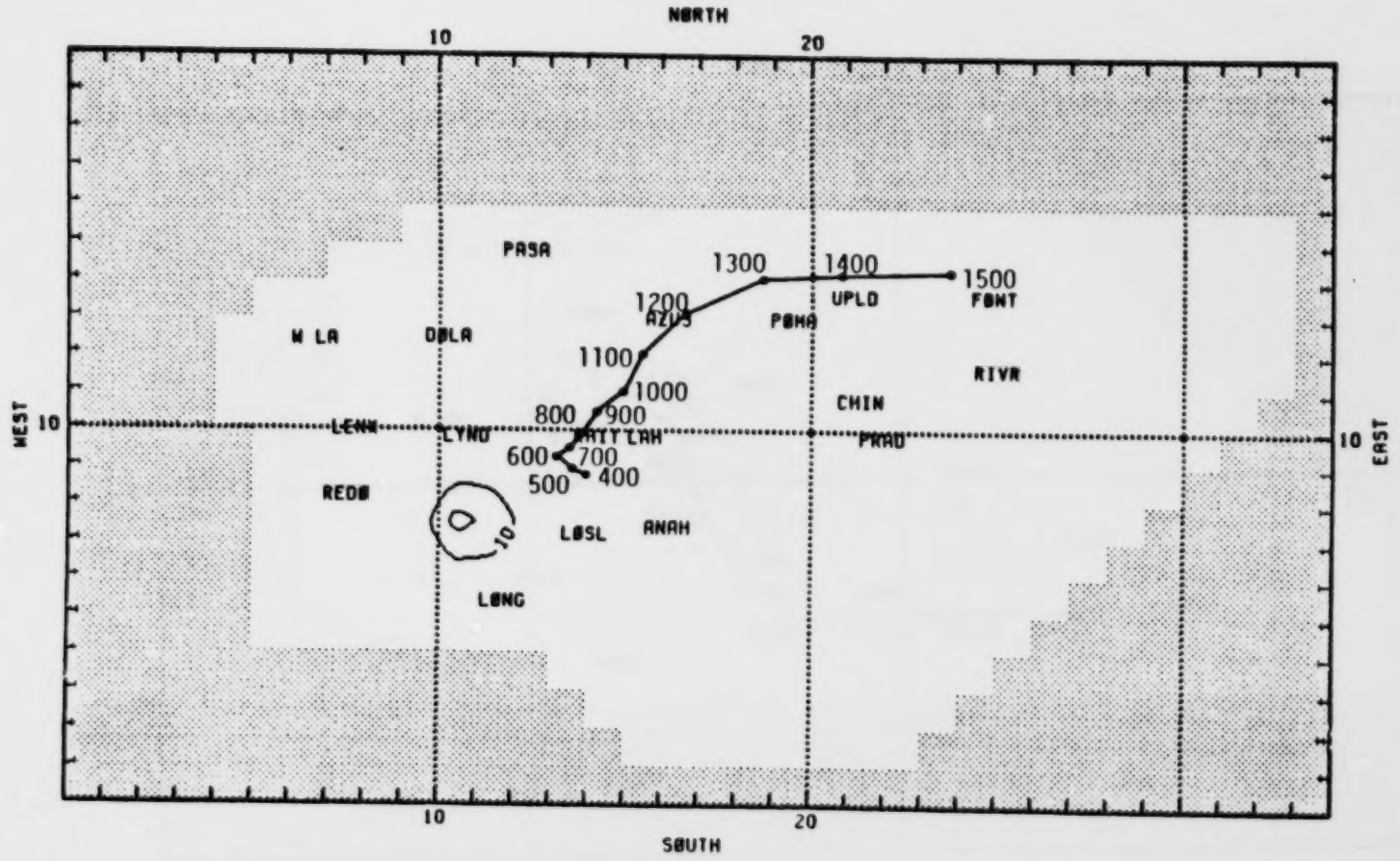


FIGURE III-3. TRAJECTORY USED IN THE EKMA STUDY OF 27 JUNE 1974

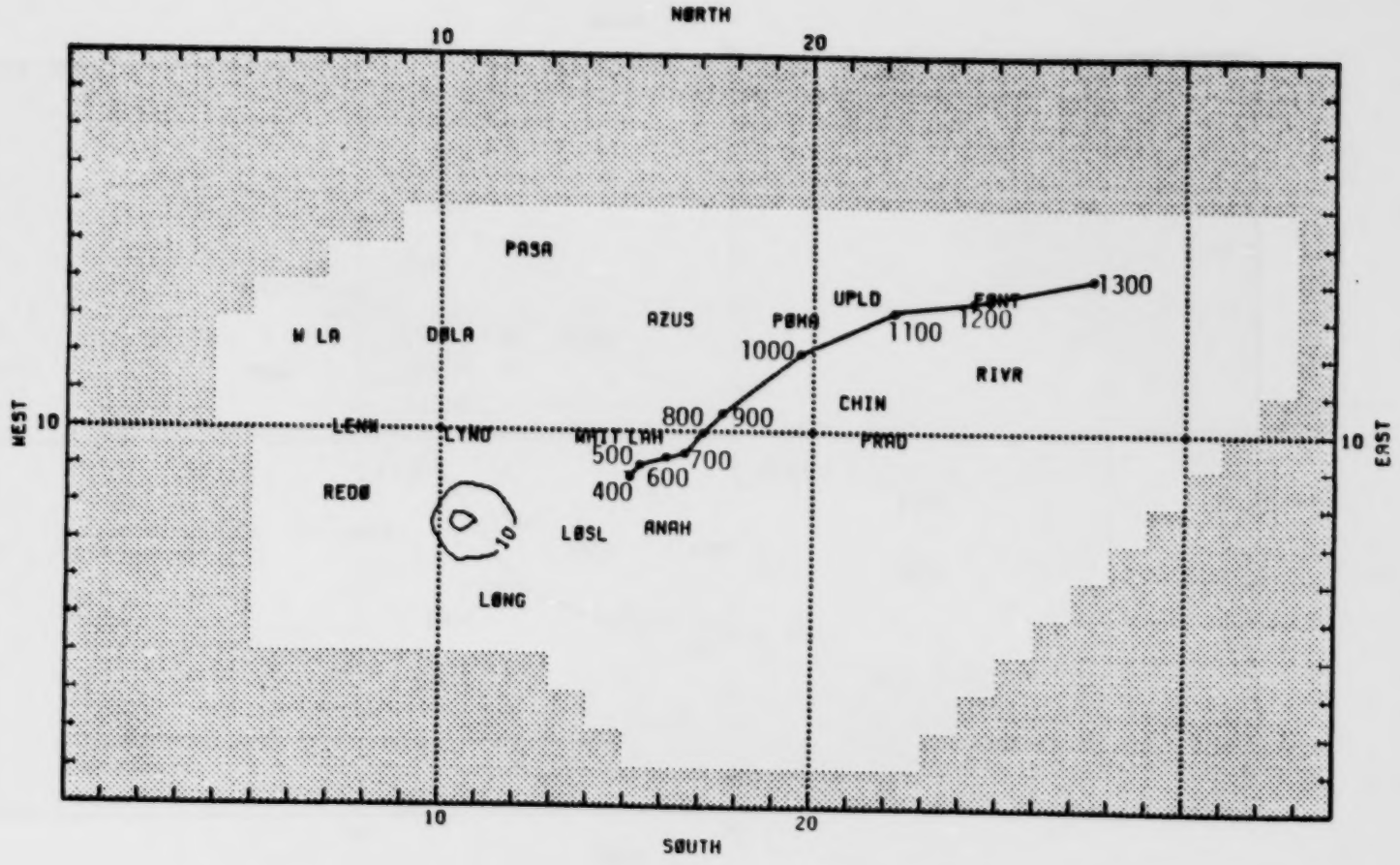


FIGURE III-4. TRAJECTORY USED IN THE EKMA STUDY OF 4 AUGUST 1975

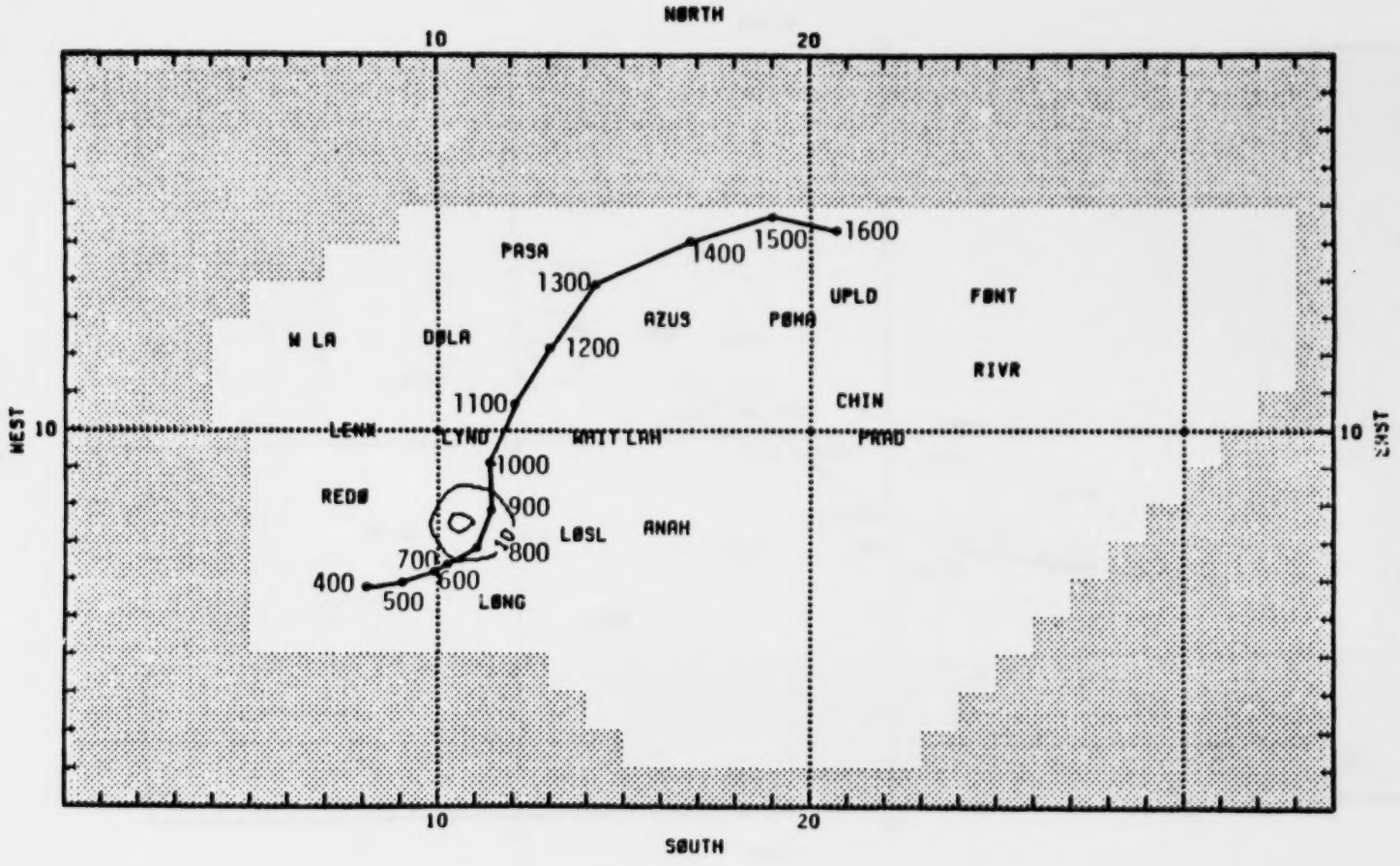


FIGURE III-5. TRAJECTORY USED IN THE EKMA STUDY OF 26 JUNE 1982

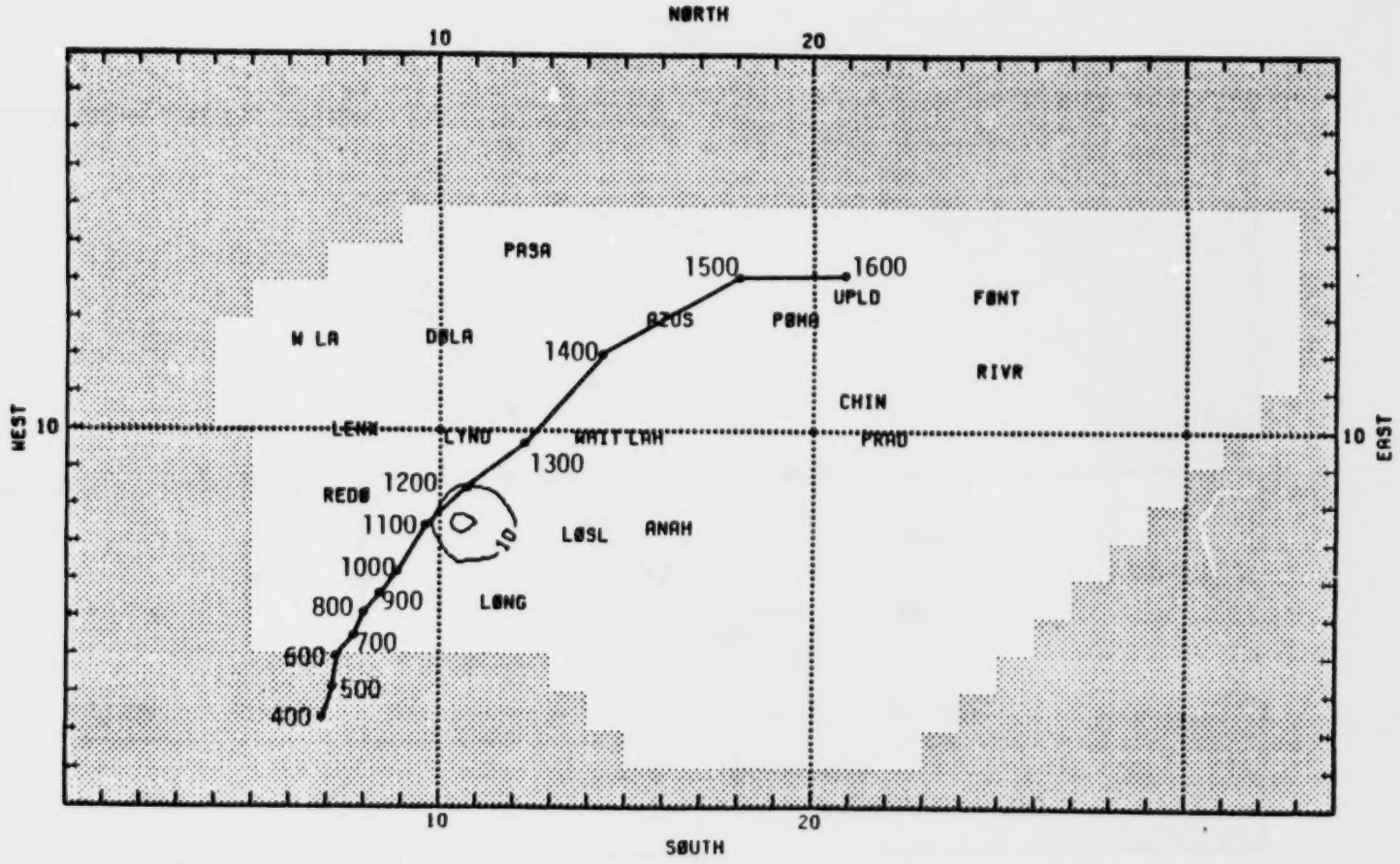


FIGURE III-6. TRAJECTORY USED IN THE EKMA STUDY OF 27 JUNE 1982

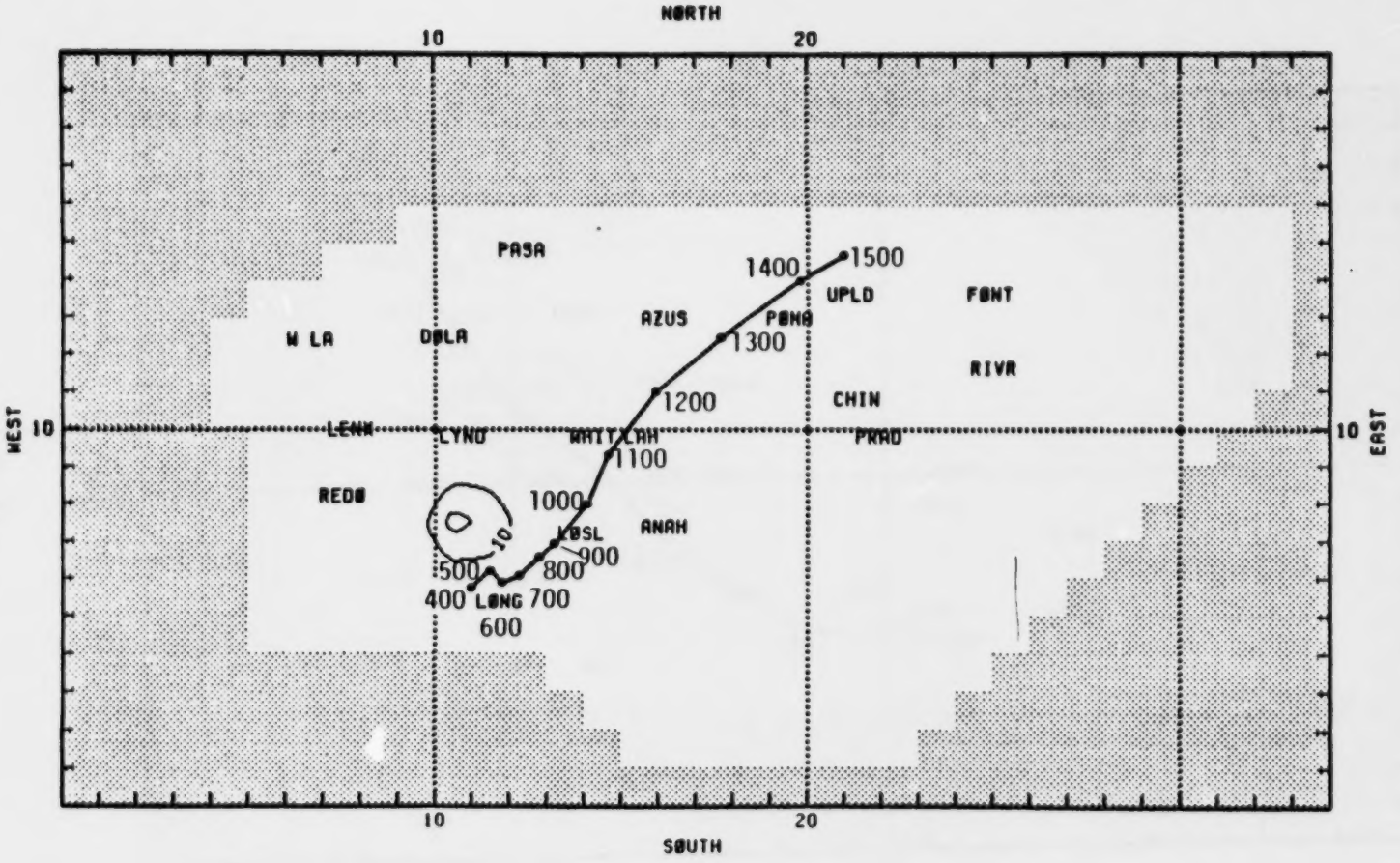


FIGURE III-7. TRAJECTORY USED FOR THE EKMA STUDY OF 4 AUGUST 1982

TABLE III-2. INITIAL CONDITIONS USED IN THE CITY-SPECIFIC EKMA*

Date	NO_2/NO_x	Surface NO_x (ppm)	Surface Hydrocarbon (ppmc)	NO_x Aloft (ppm)	Hydrocarbon Aloft (ppmc)	Surface O_3 (ppm)	O_3 Aloft (ppm)	HC/NO_x
26 June 1974	0.71	0.053	0.429	0.002	0.116	0.045	0.059	8.13
27 June 1974	0.70	0.157	0.950	0.002	0.095	0.059	0.090	6.04
4 August 1975	0.78	0.087	0.799	0.047	0.555	0.086	0.067	9.16
26 June 1982	0.77	0.042	0.256	0.003	0.117	0.050	0.08	6.06
27 June 1982	0.83	0.011	0.244	0.004	0.140	0.073	0.08	21.60
4 August 1982	0.73	0.033	0.305	0.019	0.335	0.056	0.08	9.24

* starting time = 0800 PDT

TABLE III-3. INITIAL CONDITIONS USED IN THE EKMA STUDY (CBM-EKMA MODEL)

Date	NO_2/NO_x	Surface NO_x (ppm)	Surface Hydrocarbon (ppmc)	NO_x Aloft (ppm)	Hydrocarbon Aloft (ppmc)	Surface O_3 (ppm)	O_3 Aloft (ppm)
26 June 1974	0.629	0.043	0.589	0.002	0.116	$1x10^{-9}$	0.059
27 June 1974	0.440	0.205	1.472	0.002	0.095	$1x10^{-9}$	0.09
4 August 1975	0.945	0.068	0.755	0.047	0.555	$1x10^{-9}$	0.067
26 June 1982	1.0	0.031	0.319	0.003	0.117	0.003	0.08
27 June 1982	1.0	0.020	0.381	0.004	0.140	0.01	0.08
4 August 1982	0.25	0.030	0.311	0.019	0.335	0.011	0.08

TABLE III-4. HYDROCARBON REACTIVITIES USED IN THE CBM-EKMA STUDY

Date	Hydrocarbon Fractions (surface layer)					Hydrocarbon Fractions (aloft)					Hydrocarbon Fractions (emissions)				
	OLE	PAR	ARO	ETH	CARB	OLE	PAR	ARO	ETH	CARB	OLE	PAR	ARO	ETH	CARB
26 June 1974	0.024	0.607	0.267	0.033	0.069	0.031	0.558	0.291	0.049	0.072	0.034	0.691	0.202	0.041	0.032
27 June 1974	0.021	0.632	0.253	0.027	0.066	0.01	0.30	0.31	0.11	0.27	0.034	0.684	0.208	0.041	0.033
4 August 1975	0.021	0.629	0.257	0.025	0.068	0.024	0.607	0.267	0.033	0.069	0.037	0.687	0.205	0.041	0.030
26 June 1982	0.021	0.63	0.256	0.025	0.068	0.068	0.299	0.41	0.137	0.086	0.027	0.773	0.147	0.03	0.023
27 June 1982	0.02	0.63	0.257	0.025	0.069	0.022	0.455	0.317	0.083	0.124	0.035	0.735	0.169	0.033	0.029
4 August 1982	0.021	0.63	0.256	0.025	0.068	0.03	0.567	0.285	0.046	0.071	0.031	0.69	0.211	0.039	0.029

TABLE III-5. HOURLY EMISSION FRACTIONS AND INVERSION BASES USED IN THE EKMA STUDY: 26 JUNE 1974

Time (PST)	Inversion Base (meters)	Hydrocarbon Emissions (ppmC)	NO_x Emissions (ppm)
400	100.0	0.000	0.000
500	100.0	0.105	0.029
600	127.3	0.090	0.020
700	251.0	0.169	0.042
800	297.5	0.324	0.080
900	338.9	0.327	0.089
1000	402.7	0.289	0.055
1100	499.4	0.185	0.032
1200	594.5	0.174	0.027
1300	600.0	0.129	0.034
1400	584.2	0.182	0.037
1500	518.2	0.131	0.201
1600	485.0	0.082	0.070

TABLE III-6. HOURLY EMISSIONS FRACTIONS AND INVERSION BASES USED IN THE EKMA STUDY: 27 JUNE 1974

Time (PST)	Inversion Base (meters)	Hydrocarbon Emissions (ppmC)	NO_x Emissions (ppm)
400	50.0	0.000	0.000
500	50.0	0.058	0.006
600	100.0	0.415	0.121
700	183.2	0.839	0.209
800	273.9	0.742	0.160
900	387.8	0.524	0.095
1000	471.9	0.331	0.050
1100	600.0	0.353	0.054
1200	800.0	0.261	0.057
1300	800.0	0.326	0.071
1400	800.0	0.221	0.185
1500	1000.0	0.134	0.443
1600	800.0	0.368	0.063

TABLE III-7. HOURLY EMISSIONS FRACTIONS AND INVERSION BASES USED IN THE EKMA STUDY: 4 AUGUST 1975

Time (PST)	Inversion Base (meters)	Hydrocarbon Emissions (ppmC)	NO_x Emissions (ppm)
400	290.2	0.000	0.000
500	285.6	0.007	0.003
600	270.9	0.021	0.006
700	270.3	0.055	0.014
800	255.6	0.086	0.020
900	283.3	0.054	0.011
1000	302.5	0.025	0.005
1100	310.6	0.017	0.005
1200	366.8	0.046	0.009
1300	426.3	0.035	0.074
1400	429.0	0.028	0.016
1500	429.7	0.072	0.010
1600	368.3	0.008	0.002

TABLE III-8. HOURLY EMISSION FRACTIONS AND INVERSION BASES USED IN THE EKMA STUDY: 26 JUNE 1982--DIFFERENT TRAJECTORY

Time (PST)	Inversion Base (meters)	Hydrocarbon Emissions (ppmC)	NO_x Emissions (ppm)
400	100.	0.000	0.000
500	100.	0.001	0.001
600	117.8	0.034	0.003
700	226.1	0.111	0.061
800	265.6	0.286	0.064
900	321.9	0.323	0.055
1000	414.3	0.221	0.076
1100	483.0	0.204	0.084
1200	578.7	0.188	0.054
1300	588.0	0.153	0.097
1400	589.2	0.101	0.029
1500	512.9	0.058	0.020
1600	440.8	0.015	0.007

TABLE III-9. HOURLY EMISSION FRACTIONS AND INVERSION BASES USED IN THE EKMA STUDY: 27 JUNE 1982--DIFFERENT TRAJECTORY

Time (PST)	Inversion Base (meters)	Hydrocarbon Emissions (ppmC)	NO_x Emissions (ppm)
400	50.0	0.000	0.000
500	50.0	0.000	0.000
600	50.0	0.000	0.000
700	101.8	0.00015	0.001
800	167.5	0.0004	0.004
900	228.5	0.013	0.007
1000	294.8	0.071	0.020
1100	372.8	0.200	0.340
1200	427.4	0.529	0.371
1300	481.0	0.407	0.176
1400	559.1	0.339	0.122
1500	800.0	0.194	0.060
1600	800.0	0.159	0.055

TABLE III-10. HOURLY EMISSION FRACTIONS AND INVERSION BASES USED IN THE EKMA STUDY: 4 AUGUST 1982--DIFFERENT TRAJECTORY

Time (PST)	Inversion Base (meters)	Hydrocarbon Emissions (ppmC)	NO_x Emissions (ppm)
400	204.2	0.000	0.000
500	224.6	0.003	0.005
600	189.1	0.004	0.002
700	191.4	0.002	0.00044
800	219.1	0.019	0.010
900	257.2	0.045	0.032
1000	282.2	0.054	0.024
1100	302.5	0.073	0.024
1200	346.5	0.055	0.013
1300	334.1	0.028	0.009
1400	341.2	0.037	0.015
1500	401.2	0.037	0.013

by the ratio of mixing heights used between 0400 and 0800. To some extent, the pollutant concentrations would also be modified by the concentrations assumed aloft.

Nevertheless, the main reason for starting the model earlier than 0800 is to enhance the dependence on emissions and suppress the dependence on initial conditions. Thus the general rule here would be to ensure that the contribution of the concentrations from 0400, or whatever early starting time is used, is small compared to the contribution of the emissions between 0400 and 0800, or whatever time the photochemistry begins. Critical factors to check would be the 0400 or initial mixing height as compared with the 0800 mixing height and the concentrations used aloft.

> In the present study the model comparisons are all based on common, time-dependent, gridded wind field and mixing-height sets that were generated for the SAI grid model. Any uncertainties in the preparation of these input files apply to the grid model as well as to the rest of the models used in the present study. However, the two mitigating factors associated with the slow wind speed and insensitivity to predawn mixing heights just discussed also apply to the grid model.

Although grid models have an inherent advantage over trajectory models in dealing with complex wind shear effects in the predawn hours, in actual grid model applications, the typical grid sizes used are much larger than the predawn wind shear patterns. Furthermore, monitoring data on the real wind patterns is rarely, if ever, available on a scale small enough to model the patterns precisely even if the grid size of the airshed models were small enough. Hence, in practical applications, the grid models have no real advantages over the trajectory models in their ability to handle predawn uncertainties in wind patterns and mixing heights.

> The emission density of the Los Angeles region is rather uniform over large areas; therefore, the uncertainties in wind patterns during the predawn hours do not affect the emission densities used in the models. This particular point is really an application of the general rule just discussed, namely that, especially in the Los Angeles area, the slow (in time) wind speeds combine with a slowly

rising (in space) emission density to minimize the effects of uncertainties in wind patterns.

It should be noted also that there are large differences in initial conditions among the six specific trajectories. In all cases, the values chosen came from the next highest model in the model series. For example, the initial NO_2/NO_x ratio shown in table III-3 for the CBM-EKMA on 26 June 1974 was 0.629. This number was obtained from the computer output generated by the SAI trajectory model for the time of 0400 PST. In table III-2, the city-specific EKMA NO_2/NO_x ratio for the same trajectory was 0.73, which came from the CBM-EKMA computer output at 0800 PDT.

A. A COMPARISON OF GRID AND TRAJECTORY MODELING RESULTS

We first compare the results of the SAI grid model and the SAI trajectory model. Because the only possible difference in results along the trajectory paths must be due to the result of horizontal dispersion and dilution effects (the two models are identical except in concentration changes caused by horizontal effects such as convergence), the large difference in results for some days (notably 26 June 1974, 4 August 1975, and 27 June 1982) is striking. The maximum observed ozone concentration occurs in Fontana for the first two of these days and the grid model results show poor agreement with observations, whereas the trajectory models all show at least fair agreement with the observations.

Comparison of the results produced by the two models for these two days illustrates a very important point about the use of sophisticated grid models--that is, trajectory models provide a diagnostic tool useful in understanding discrepancies between observations and grid-model simulations. In the present case, a review of grid model intermediate results revealed that the low simulated ozone values for Fontana are significantly affected by wind shear effects computed from the topographic influences of the steep mountains nearby. Evidently, the grid-model wind field algorithm leads to unrealistically high dilution. Since such effects are ignored in the trajectory models, it appears that for grid cells so affected the grid-model results are less dependable.

The 27 June 1982 trajectory illustrates a somewhat different problem. The grid-model simulation predicts a rather high ozone level because of a high (0.3 ppm) ozone concentration aloft near Upland. The ozone is entrained when the mixing layer thickens in the afternoon. The high ozone aloft originates several grid squares away, where a simulated wind-flow convergence zone pushes polluted air aloft. This air is, in turn, carried to the Upland region by the winds aloft. Since the winds aloft are not parallel to the surface winds, the trajectory model entrains much cleaner

air, using the same inversion rise as the grid model. In fact, the ozone in the trajectory model is diluted during the period in which air along the same path in the grid model is enhanced by ozone from the air aloft. However, the impact of the ozone aloft may be exaggerated in this case because of a questionable feature of the grid model mixing-height algorithm. This feature is now being investigated, partly as a result of the present comparison study.

Trajectory models cannot normally simulate important effects such as wind shear. In one case we found a method for coping with this effect. Two values are shown in table III-1 for the 4 August 1982 SAI trajectory mModel simulation at Upland. The value in parentheses was obtained by considering elevated point sources. The other value ignores elevated point sources for this trajectory as do the values from all the EKMA-type models for this particular day. There was a substantial wind shear through the mixing layer up to 1000 hours in the morning for this particular trajectory. At the same time, the atmosphere was only moderately unstable in the cool mixing layer. These two effects of wind shear and minimal mixing combine to force the elevated NO_x emissions down to the side of the trajectory path modeled. Of course this effect is exaggerated to some extent in the present algorithms because the path of the trajectory model is defined by only the surface-layer wind field of the grid model.

Some sophisticated averaging process might have been used for the grid model layers below the mixing height, based on such factors as the vertial mixing rate and wind speed, to determine an alternate trajectory path. In this case, a partial treatment of the elevated sources might have been more appropriate. However, the success of the simple treatment of the trajectory path and the simple solution of ignoring the elevated sources seemed to preclude the need for any further improvements during the present study. Nevertheless, a concurrent study at SAI has encountered a severe wind-shear day in the Sacramento region that does not respond to the simple ignorance of elevated sources, so that averaging of the vertical wind fields has been necessary to generate reasonable simulations.

Incidentally, the trajectory model simulations imply that the site of maximum simulated ozone at Upland for this day could result from the presence of wind shear below the mixing height. The absence of wind shear would apparently allow the elevated NO_x emissions to suppress ozone along the trajectory path.

B. A COMPARISON OF CBM-EKMA AND SAI TRAJECTORY MODELING RESULTS

The nine pairs of results shown in table III-1, which compare the SAI trajectory model with the CBM-EKMA, show agreement to a standard deviation of less than 8 percent. Considering the many differences between these two models this agreement appears to indicate that the most important features of the more complex trajectory model are reasonably represented in this CBM-EKMA. Future studies might create more models between these two variations for purposes of investigating additional model features. As an example, model results have been found to be sensitive to temperature. In a recent study, which used a different Los Angeles trajectory than any reported in this work, it was found that the same EKMA, used with CBM chemistry, produced 0.41 ppm ozone when run at a constant 305 K and 0.38 ppm ozone when run at a constant 300 K (Whitten and Hogo, 1980).

Temperatures in the SAI trajectory model typically vary between about 290 K and 314 K in the course of a simulation. An overall impression, gained from comparing the detailed outputs of the SAI trajectory model and the CBM-EKMA, is that the formation rate of ozone in the morning hours is usually somewhat faster in the CBM-EKMA than in the SAI trajectory model; however, the situation reverses in the afternoon. This effect would be consistent with the constant temperature used in the EKMA, which is higher than the morning temperatures used in the SAI trajectory model and which is lower, of course, during the afternoon. This overall impression of the relative rates of ozone formation is opposite to the behavior that is normally expected as a result of differences such as steady-state approximations versus full Gear-type simulations and differences in the aldehyde photolysis rate.

A very brief investigation of diurnal emission patterns was made for the 26 June 1982 simulation based on the 1974 path. Two values are shown in table III-1: the value shown in parentheses was computed using the 1974 pattern of emissions; however, the emissions levels were uniformly reduced to reflect the reductions along the total path. The regular value was computed directly from the 1982 emissions files of the SAI grid model, as were all other 1982 values shown in table III-1. Since the results differ by only 5 percent, the pattern change was only moderately important.

The CBM-EKMA model results originally showed the largest difference from results of the SAI trajectory model for the trajectory to Upland of 27 June 1974. Although observed maximum ozone of 0.49 ppm occurred at Upland that day, the SAI grid and trajectory models both simulated only 0.32 ppm ozone, whereas the CBM-EKMA originally simulated only 0.28 ppm ozone. After a considerable effort was made to understand the main reasons for the discrepancy, it was discovered that carbon monoxide levels

in the SAI trajectory model have a significant influence on ozone production. The ozone result shown (0.30) for the CBM-EKMA in table III-1 includes CO emissions in order to bring the CO levels close to the values seen (approximately a 3 ppm average) in the SAI models.

To estimate the importance of physical dispersion differences between the SAI trajectory model and the modified CBM-EKMA we operated both models without chemistry. The comparison data for 27 June 1974, are presented in table III-11. Data for ethylene (ETH) and the single-bonded carbons (PAR) are not completely comparable because the reactivity (splits between the various CBM species) varies with time in the SAI trajectory model but is constant in the EKMA. The overall similarity indicates that such factors as multiple levels, eddy-diffusion, and variable reactivity are not critical for this trajectory.

Since the results of the runs with chemistry are similar for all of the comparisons shown in table III-1, it is tempting to speculate that the multiple levels, eddy-diffusion, and variable reactivity treatments are never very important. However it is probably better to determine for each specific case to be considered in the future whether or not any of these treatments appear to be especially important. For instance, variable reactivity would be an especially important treatment if a large new source was to be considered along the trajectory path and if the hydrocarbon reactivity of this source was considerably different from the average of the existing sources.

C. CHEMICAL MECHANISM COMPARISON RESULTS

A comparison of chemical mechanisms appears to show that significant differences can occur as a result of the different model chemistries. Three columns of results in table III-1 compare the EKMA trajectory models that differ only in chemistry. The first two of these columns compare the CBM-EKMA with the propylene/butane-EKMA, which had equal photolysis rates. The next two columns compare the same propylene/butane chemistry with and without the adjusted photolysis rates. Figure III-1 shows some of the same comparisons.

Some trajectory runs were also made adjusting only NO_2 photolysis (up by 13 percent), but with standard EKMA aldehyde rates (3 times higher than used in the CBM). Virtually no difference was found for the peak ozone values when the results were compared to the fully adjusted photolysis results, yet the ozone level did begin to rise much earlier in the day. Some trajectory runs were also tried using higher reactivities for the propylene/butane emissions mix (propylene percentages up to 35 were used). Again, the ozone level rose earlier in the day but the maximum

TABLE III-11. A COMPARISON OF THE SAI TRAJECTORY MODEL AND THE EKMA: 27 JUNE 1974

(a) NO_x Concentrations

Time (PST)	Trajectory Model (ppm)	EKMA Model (ppm)
400	0.043	0.043
500	0.071	0.072
600	0.072	0.073
700	0.055	0.055
800	0.074	0.073
900	0.091	0.089
1000	0.091	0.088
1100	0.087	0.078
1200	0.073	0.071
1300	0.078	0.077
1400	0.085	0.084
1500	0.124	0.122

(b) ETH Concentrations

400	0.0096	0.0096
500	0.0124	0.0118
600	0.0132	0.0124
700	0.0119	0.0116
800	0.0130	0.0132
900	0.0143	0.0144
1000	0.0147	0.0148
1100	0.0142	0.0138
1200	0.0139	0.0125
1300	0.0143	0.0129
1400	0.0148	0.0135
1500	0.0157	0.0139

(c) PAR Concentration

400	0.358	0.358
500	0.442	0.430
600	0.406	0.395
700	0.268	0.265
800	0.304	0.303
900	0.338	0.333
1000	0.340	0.336
1100	0.307	0.300
1200	0.284	0.280
1300	0.298	0.291
1400	0.320	0.314
1500	0.337	0.329

ozone level was not significantly affected. Evidently the CBM chemistry produces more ozone for amounts of emitted HC late in the day than does the propylene/ butane chemistry.

Comparison of either the CBM-EKMA or models using propylene/butane chemistry with observed data would not provide an appropriate assessment of the quality of the chemical mechanisms. Mechanism comparisons must be done at many levels and should include these considerations:

- How well do the basic reactions of each mechanism compare with known and evaluated reactions? For example, the propylene/butane mechanism uses a value for the rate constant of the HO_2 reaction with NO that is low compared with recent evaluations.

- How important are the reactions that are not updated? For instance, it was found that updating the reaction rate constant for the HO_2 reaction with NO in the propylene/butane mechanism tended to remove most of the difference between its results and those obtained with the CBM-EKMA for the late afternoon period discussed earlier.

- How well do the mechanisms simulate a set of smog chamber experiments covering a wide range of concentrations and HC/NO_x ratios?

- How well do the mechanisms treat the conversion of atmospheric species into the surrogate species utilized in the mechanisms?

- How well do the mechanisms respond to differences in reactivity?

Once a mechanism has been put into an atmospheric model and used to simulate a specific situation, a large number of elements are introduced that can either compensate or add to deficiencies in the chemistry. Therefore, a comparison of mechanisms with observed data in such cases is inappropriate except as an additional element to be considered along with the comparisons just discussed.

More investigative work in the area of mechanism comparison is needed; however, other consistent explanations exist, in addition to the reaction updating just mentioned, that might eliminate the ozone peak discrepancy between the propylene/butane mechanism and the CBM. For instance, the CBM chemistry has a more balanced distribution of reactivity that the propylene/butane mix cannot simulate. When the propylene used in

the standard EKMA has virtually all reacted, the remaining butane is too unreactive to maintain a significant rate of ozone buildup. The detailed computer outputs showed that the propylene fraction remaining often fell below 5 percent between 1200 and 1500 hours, meaning that 95 percent of the remaining HC consists of butane. The CBM, however, uses additional species, with intermediate reactivity such as ethylene and aromatics that provide a more constant rate of ozone buildup.

The effect observed in this study does not appear to be as simple as either of the explanations given because dilution, continuous emissions, HC/NO_x ratio, and overall concentration all seem to interact differently with the two mechanisms. For instance, the 1982 results are much closer in agreement for the three pertinent columns of table III-1 (columns 4, 5, and 6) than for the base-case years (1974 and 1975). In addition to the implication of involvement of HC/NO_x ratios and concentrations, the control-strategy predictions for the two chemistries can obviously be different. This point will be discussed later.

D. COMPARISON OF LINEAR AND EXPONENTIAL MIXING-HEIGHT RESULTS

Study results obtained from a comparison of dilution determined from linear interpolation of hourly mixing-height input data, and from exponential interpolation of only two mixing heights are not significantly different. For this particular series of trajectories the temporal behavior of the mixing heights closely resembled the exponential curves implicit in the regular EKMA. The most significant difference in the mixing-height comparison columns of table III-1 occurred for the trajectory of 27 June 1982 in which the standard model, using the exponential curve, predicted 0.07 ppm ozone compared to a prediction of 0.11 ppm ozone for the more sophisticated model, which used hourly mixing-height inputs. Figure III-8 shows the temporal behavior of mixing heights for this case.

E. COMPARISON OF THE CITY-SPECIFIC EKMA WITH THE STANDARD EKMA RESULTS

The results of the final comparison shown in table III-2 contrast the city-specific model with the model used to generate the standard EKMA isopleth diagram. This comparison involves several differences in model input data. In general, initial aldehyde and ozone concentrations, pollutants aloft, post-0800 emissions, and initial NO_2/NO_x ratios all favor ozone production for the city-specific model in contrast to the standard EKMA isopleth version. However, similarities and differences in the results of these two versions are most easily explained by differences in the mixing heights used by the city-specific model. The standard EKMA

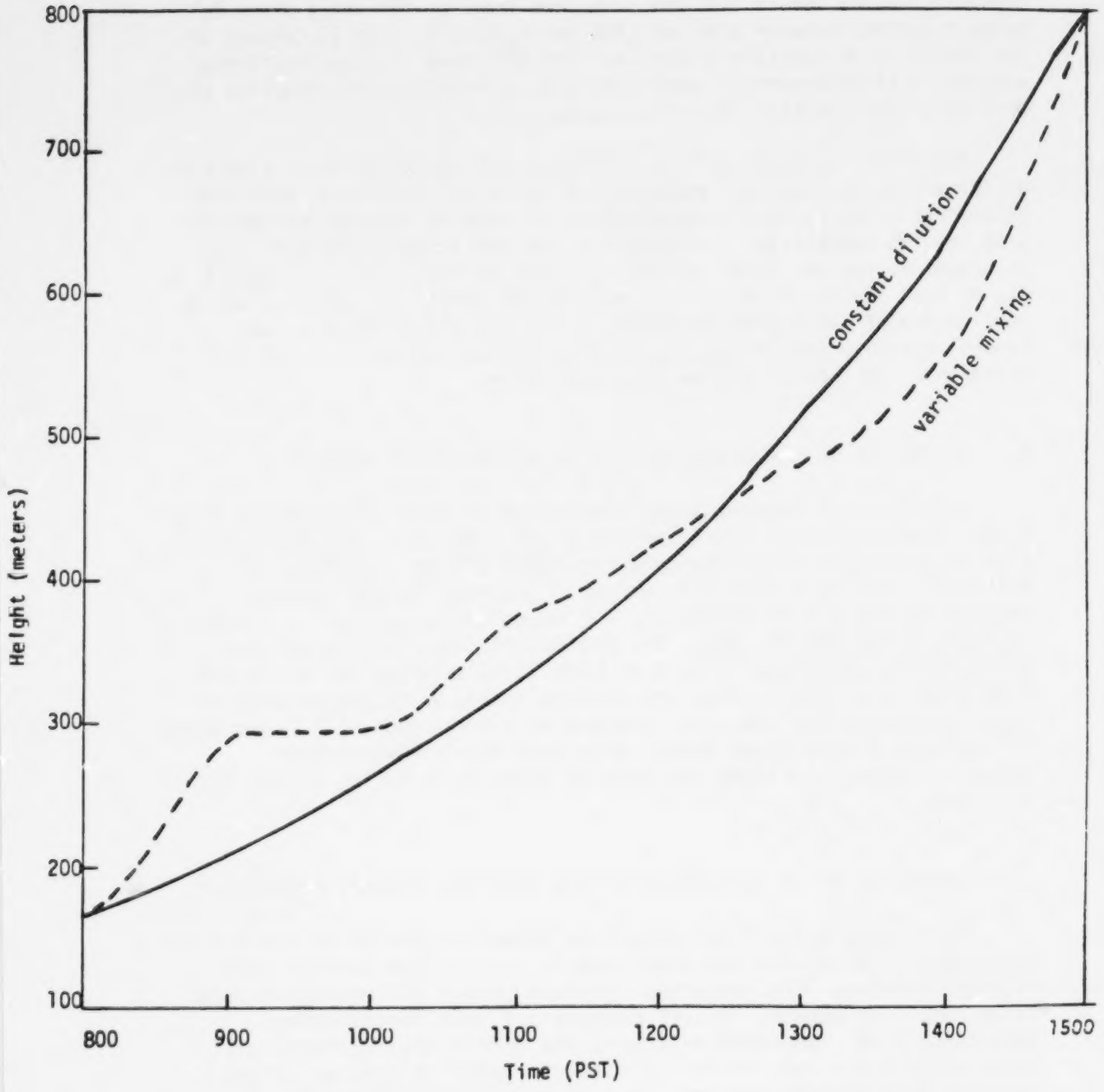


FIGURE III-8. COMPARISON BETWEEN CONSTANT DILUTION AND VARIABLE DILUTION RATE FOR 27 JUNE 1982

isopleth assumes a mixing-height change of 24 percent, whereas the city-specific simulations use changes of 58 to 365 percent. The city-specific model allows mixing-height inputs that correspond to morning and afternoon levels. Hence the city-specific model predicts higher ozone levels because of the many effects noted above than does the standard model if the mixing-height changes are relatively small through the day.

For 4 August 1982, the mixing-height change was the smallest for this series, giving a predicted ozone level of 0.20 ppm, compared to 0.13 ppm for the standard EKMA. For this case, when the change in mixing height was large, the city-specific model actually predicted lower ozone concentrations than did the standard model. For the 27 June 1974 trajectory, the change in mixing height was 265 percent, giving a predicted ozone concentration of 0.21 ppm, compared to the standard model ozone prediction of 0.24 ppm. This mixing-height explanation is not complete, however. The comparison for 27 June 1982 is more appropriately explained by the ozone concentration aloft because the mixing-height change was very large (365 percent); yet the two models predicted similar ozone levels near 0.06 ppm--the ozone concentration aloft in the city-specific model was 0.081 ppm for this case.

IV THE USE OF ISOPLETH DIAGRAMS TO PREDICT OZONE LEVELS

The EKMA uses ozone isopleth diagrams according to a specific set of guidelines to estimate control scenarios that should produce ozone reductions sufficient to meet federal or state standards. The isopleth diagrams themselves are constructed according to a set of assumptions by computer simulation of many individual precursor-emissions combinations, using the same trajectory model and trajectory path.

In the previous sections we compared an EKMA trajectory model to the more complex SAI trajectory model and to the SAI Urban Airshed Model. Using computer programs OZIPP and OZIPM, it is possible to construct ozone isopleth diagrams from many repeated individual applications of any of the models previously discussed. In this section we explore some of the assumptions used in the construction and application of isopleth diagrams in the EKMA. In addition, we offer some suggestions that may improve the reliability of this modeling approach.

Isopleths based on EKMA trajectory models create some uncertainties when used to predict the maximum observed ozone levels that result from changes in precursor emissions. These uncertainties are inherent either in the nature of the models themselves or in the assumptions necessary to construct the isopleth diagrams. Some of the factors involved are:

- Fixed monitoring sites--As discussed earlier, the time and location of maximum observed ozone concentrations might change as a result of a change in emissions. Unless the wind direction is constant, air arriving at a monitoring site at different times of the day can originate from quite different locations. Thus, the trajectory path to a monitoring site may be much different at different times. Often, some areas of an urban airshed have different HC/NO_x ratios and concentrations from those of the trajectory path that lead to the site of maximum observed ozone. Application of even a uniform emissions control policy could conceivably lead to different degrees of improvement (if not deterioration) in other areas of the airshed. Therefore, the location of the monitoring site at which maximum observed ozone occurs may vary in future years.

- Uneven changes in emissions--Mobile-source emissions are, for the most part, regulated at the federal level, yet stationary sources are usually subject to local control. Therefore, the uniform control of either HC or NO_x is rarely even in time and space. Although individual trajectory-model simulations might provide acceptable levels of accuracy for the base-case year and the future year, the isopleth approach is not readily adaptable to nonuniform emission changes.

  Under the present algorithms, each isopleth diagram must use the same emission pattern for the entire diagram. However, the impact of alternate emission patterns can be estimated by changing the pattern and generating a new set of isopleths. Thus, non-uniform emission changes could be handled through an iterative process in which the amount of necessary average control is first estimated on the original diagram. Then, a new diagram is constructed on the basis of the pattern projected for realistic implementation of the first estimate. Next, any corrections resulting from the changes in the emission pattern are reintroduced on the original diagram. Finally, a third diagram could be constructed if the expected emission pattern was significantly different from that used in the second diagram. The process would then be repeated until the combined precursor reductions and emission pattern changes resulted in the desired ozone level.

  Another method for dealing with the problem of interaction between federal mobile-source control and local stationary-source control has been suggested. This approach first involves the construction of an isopleth diagram in which every point has an equal contribution of stationary sources in the absolute sense. Such a diagram would supposedly characterize the response to mobile-source controls only; then, an estimate of changes in vehicle-mile reductions and mobile emission reductions for some future year should produce an estimated future ozone level on the diagram using the normal EKMA method. Next, a second diagram would be constructed in which every point corresponds to the estimated future mobile emissions; this second diagram would supposedly characterize the response to stationary-source controls. The local air pollution management district could then base their local control estimates on this second isopleth diagram.

> Transported pollutants--As seen in this study, assumptions that are used for pollutant concentrations aloft, or that are found in the initial conditions, can significantly affect simulated maximum ozone results based on future emissions scenarios. The grid-model simulations used in this study were purposely intended to be conservative estimates of air quality improvement. Hence the pollutant levels in the air aloft were not rolled back with emissions reductions. The initial (i.e., 400 PST) conditions were also not rolled back in the 27 June 1982 simulation.

A key feature of the EKMA when isopleth diagams are involved is the relative nature of this approach. Whether or not the trajectory model involved simulates the absolute ozone concentration at the point of the isopleth where one begins is not important to the use of the EKMA. To be sure, a gross lack of agreement in the absolute sense would be of primary concern regarding the ability of the combination of model and input data to appropriately simulate relevant atmospheric conditions. Nevertheless, the inherent "calibration" or adjustment involved when the model is fixed at the starting point on an isopleth diagram eliminates many minor problems associated with atmospheric monitoring and modeling. This simple and straightforward adjustment feature of the EKMA provides a distinct advantage over a complex airshed model in predicting control implications. When complex airshed models don't quite agree with the base case air quality data, it is difficult to predict future air quality. This fact is by no means an indication of the quality or appropriateness of these two types of models. The complex models have many adjustments in their input files that can be justified within some range, and straightforward calibration procedures have yet to be established.

A. COMPARISONS OF ISOPLETH PREDICTIONS

In this section, predictions obtained using the EKMA isopleth diagrams are compared with the predictions based on the SAI grid and trajectory models. Since the isopleth method normally involves predictions that utilize base case observations, the observed data is also used. However, appropriate comparisons, starting with observed data, can be made only between the various EKMA-type models because the SAI grid and trajectory models do not have the calibration feature of the isopleth approach.

The emission files used in the Airshed Model study form the basis for the percentage emission changes shown in table IV-1. Those trajectories discussed in section III were used. However, as shown in table IV-1, a

TABLE IV-1. PERCENTAGE OF EMISSION CHANGES

Date	Total Area		Specific Trajectory	
	HC	NO_x	HC	NO_x
June 26 74 → 82	-47	-21	-48	-17
June 27 74 → 82	-44	-19	-49	-15
August 4 75 → 82	-47	-20	-50	-14
June 26 82 → 74	+87	+27	+84	+20
June 27 82 → 74	+79	+23	+98	+14
August 4 82 → 75	+89	+25	+99	+24

new comparison, based on a total emission inventory for the entire gridded area, is also included because percentage changes in emissions for the total area are commonly used with the EKMA. Although the specific trajectory paths are the same as those discussed in the previous sections, the changes in emissions shown in table IV-1 are percentage changes for the total trajectory. In work described in the previous sections, the 1982 initial conditions and hourly emission inputs were taken from the model used for specific comparison, as just discussed. For the isopleth predictions, the initial conditions, reactivity, and diurnal changes in emissions must always be derived from the base case values unless separate isopleth diagrams are used for the predicted values. Hence, those percentage changes shown in table IV-1 that are based on 1982 data imply that the base case values for trajectory reactivity and diurnal emissions also came from the 1982 specific trajectory model.

The order of discussion of the EKMA models does not follow the order of the model series presented earlier. This change was made because the modified EKMA-type models were used with a different style of isopleth diagram that is more appropriately introduced later in this section. The isopleths generated for the regular city-specific EKMA model, using the unmodified OZIPP computer code, are presented in figures IV-1 through IV-6 for the six specific trajectories used in this study. Figure IV-7 is the so-called "standard" EKMA or Level IV diagram. In addition to the isopleth lines generated by the OZIPP computer code, figures IV-1 through IV-7 contain several lines and special points of interest that are explained below.

The isopleth diagrams were used in several different ways to allow comparisons among the various models used in this study. In the previous sections the model comparisons involved steps in a series. Thus, a given model could be properly compared only with adjacent models in the series. However, the calibration feature of the isopleth diagrams as used in EKMA enables us to calibrate any one model to observed data or to any other model. On the other hand, prediction comparisons of specific calculations between series-adjacent models in section III involved parameter changes between base and predicted simulations that cannot readily be incorporated into single-isopleth diagrams. As discussed previously, examples of these parameter changes are reactivity and diurnal emissions patterns. When a grid model is compared with a trajectory model, the change could be in the trajectory path itself if maximum ozone predictions form the bases of comparison.

Figures IV-1 through IV-6 typically show two HC/NO_x ratio lines; 3 points labeled 1,2, and PREDICTED O_3; an AIRSHED-PREDICTED O_3 point along each HC/NO_x ratio line; and an OBSERVED O_3 point on the solid HC/NO_x ratio line. Figure IV-7 is divided into three parts; each part has points labeled 1 to 6 and three ratio lines on which the design O_3 is indicated.

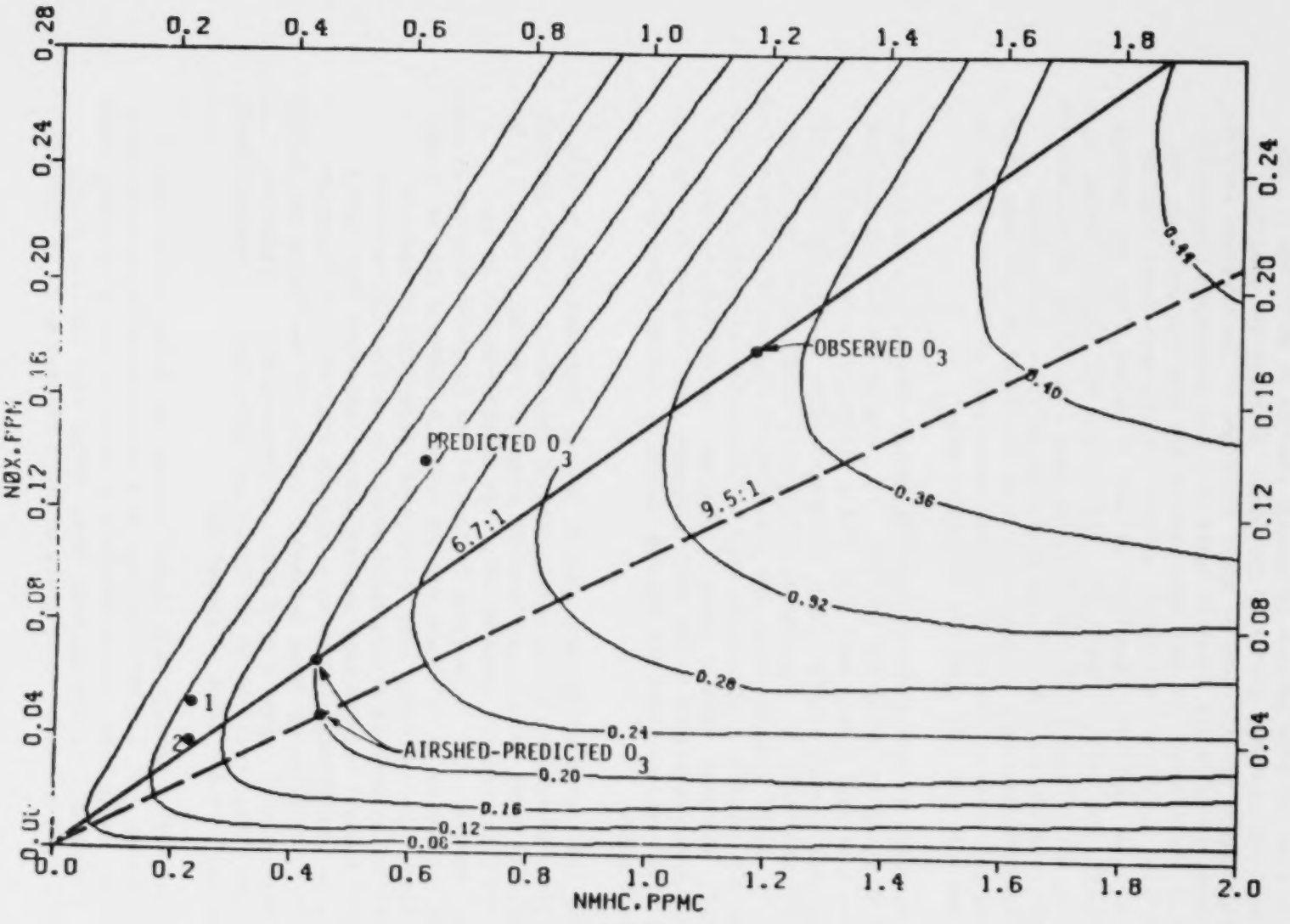


FIGURE IV-1. STANDARD OZIPP RUN (CITY-SPECIFIC EKMA) FOR 26 JUNE 1974

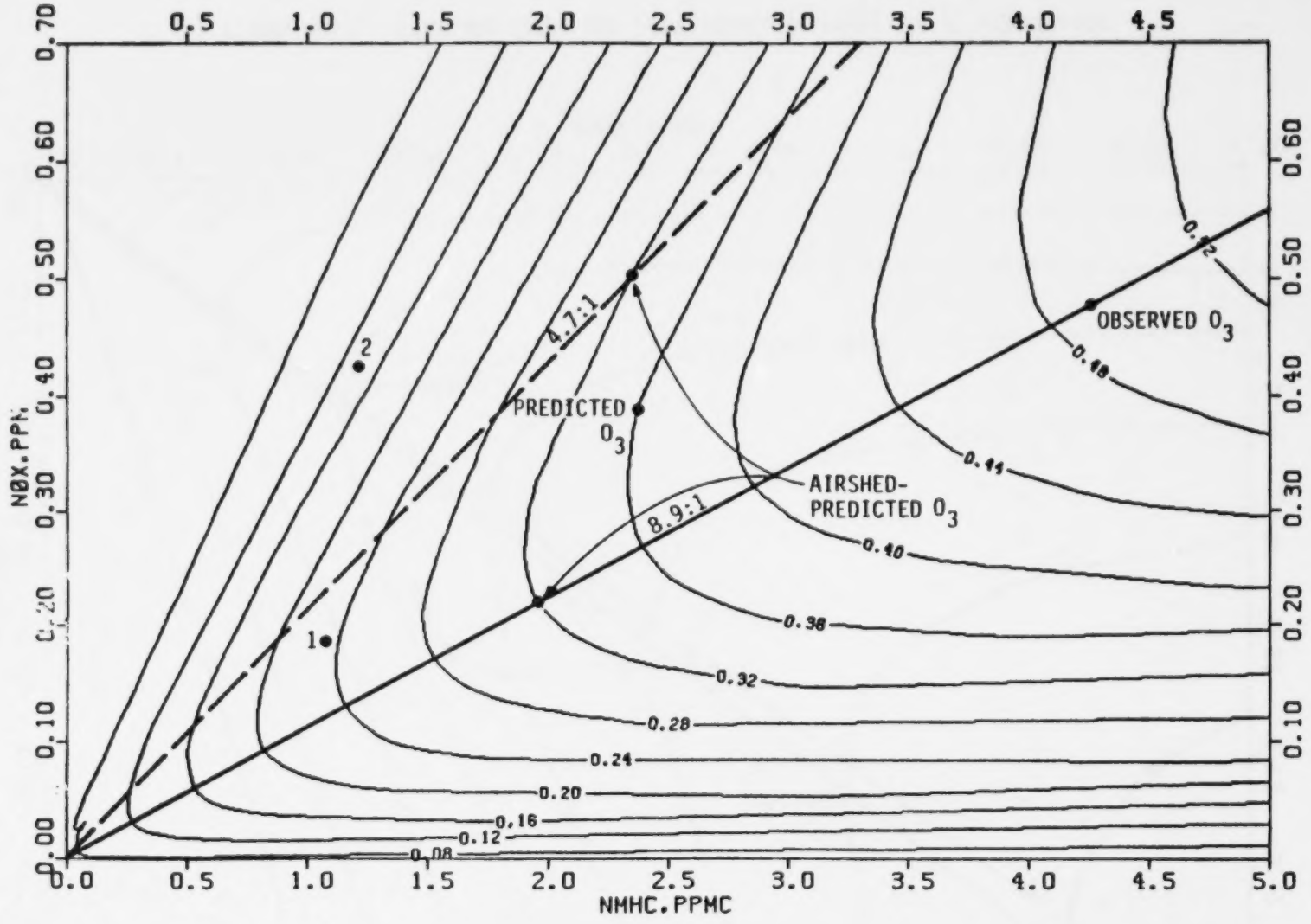


FIGURE IV-2. STANDARD OZIPP RUN (CITY-SPECIFIC EKMA) FOR 27 JUNE 1974

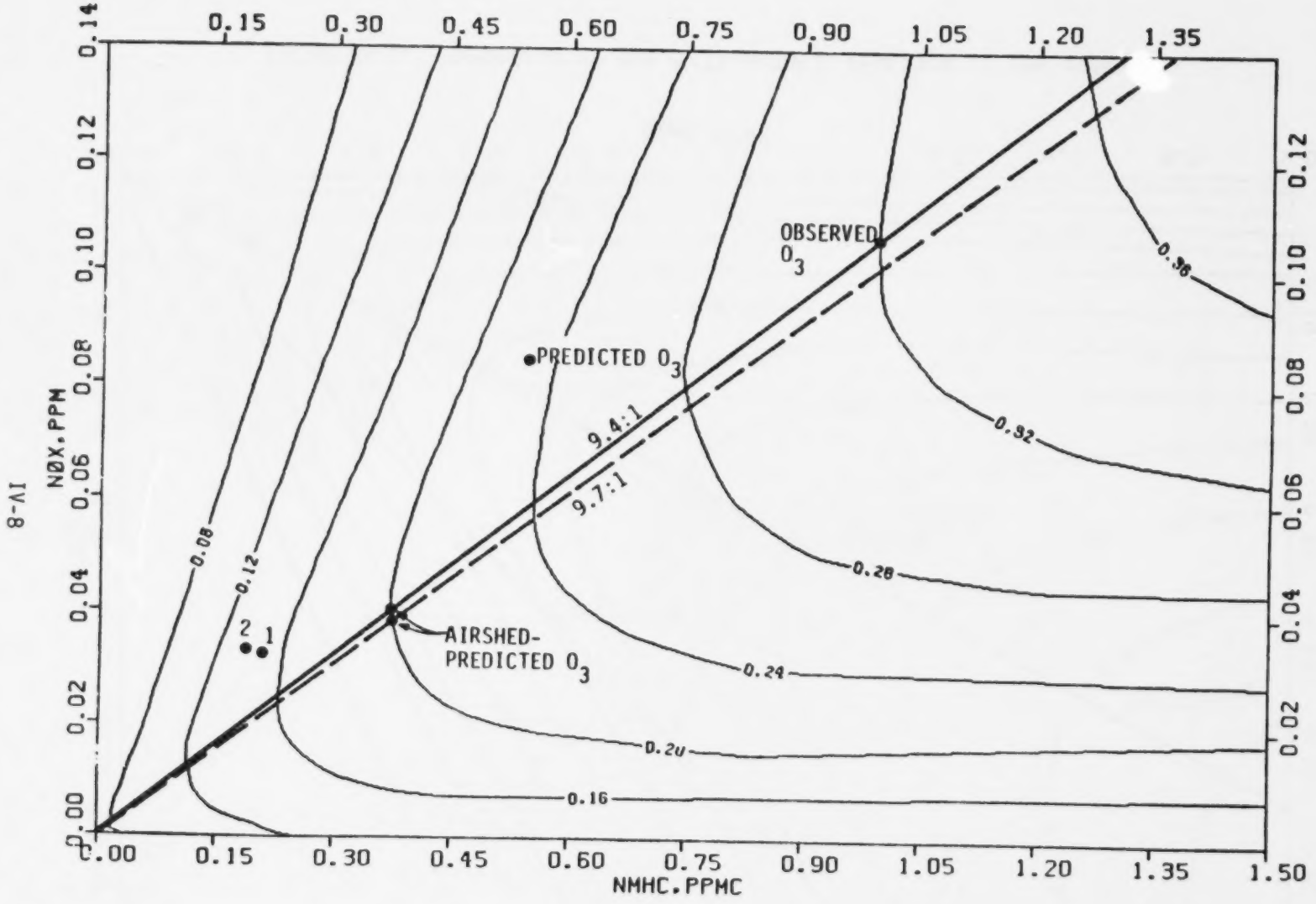


FIGURE IV-3. STANDARD OZIPP RUN (CITY-SPECIFIC EKMA) FOR 4 AUGUST 1975

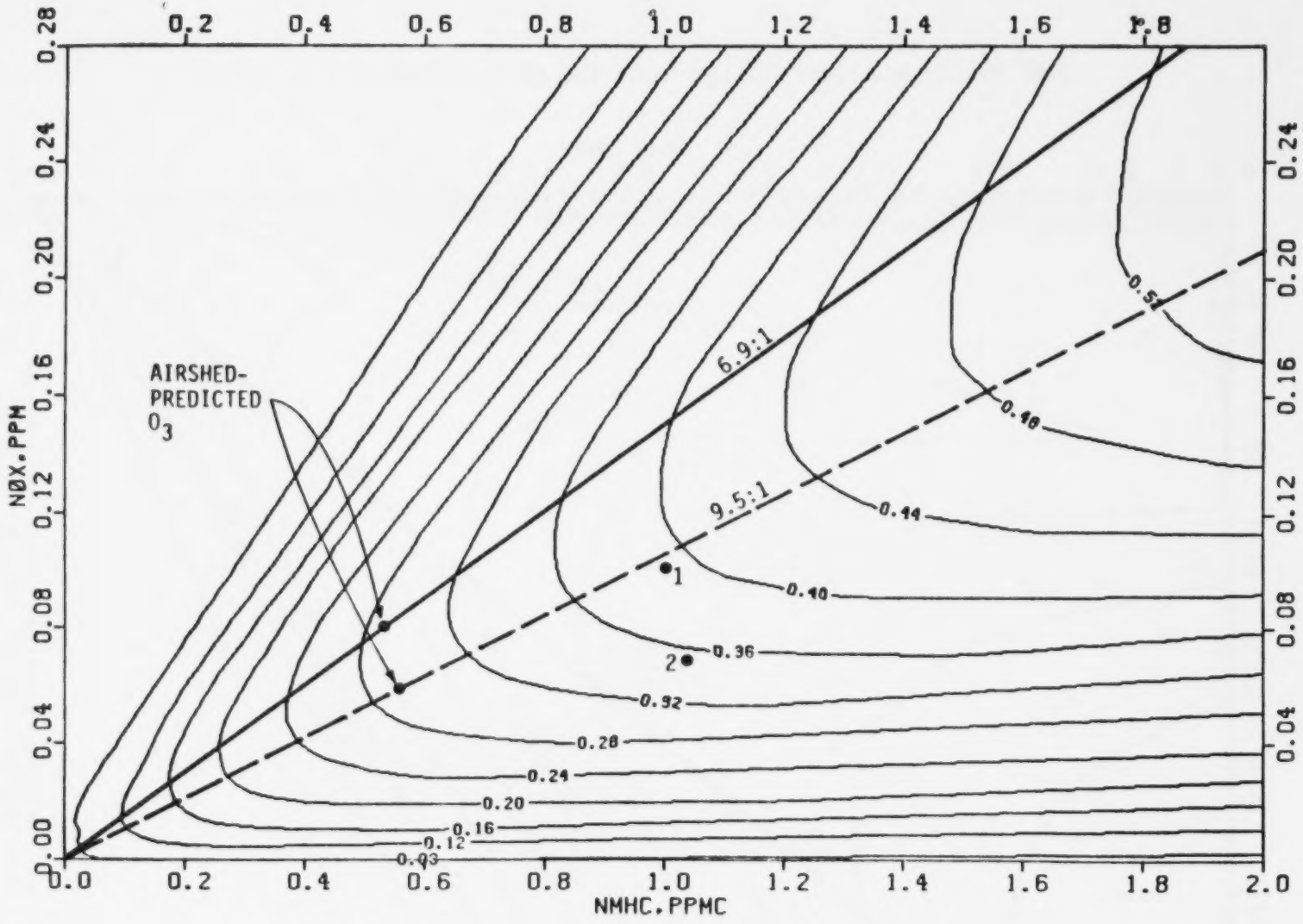


FIGURE IV-4. STANDARD OZIPP RUN (CITY-SPECIFIC EKMA) FOR 26 JUNE 1982

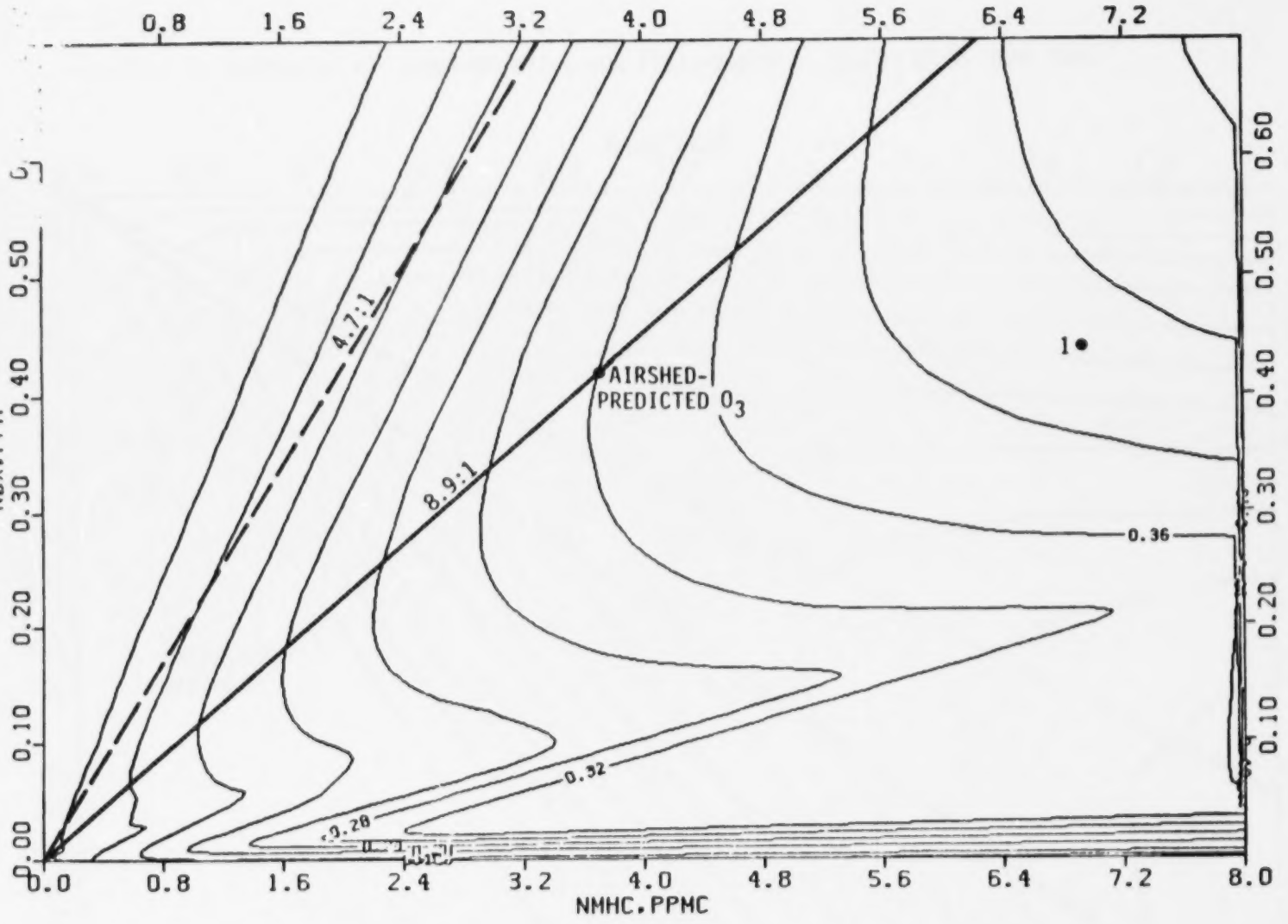


FIGURE IV-5. STANDARD OZIPP RUN (CITY-SPECIFIC EKMA) FOR 27 JUNE 1982

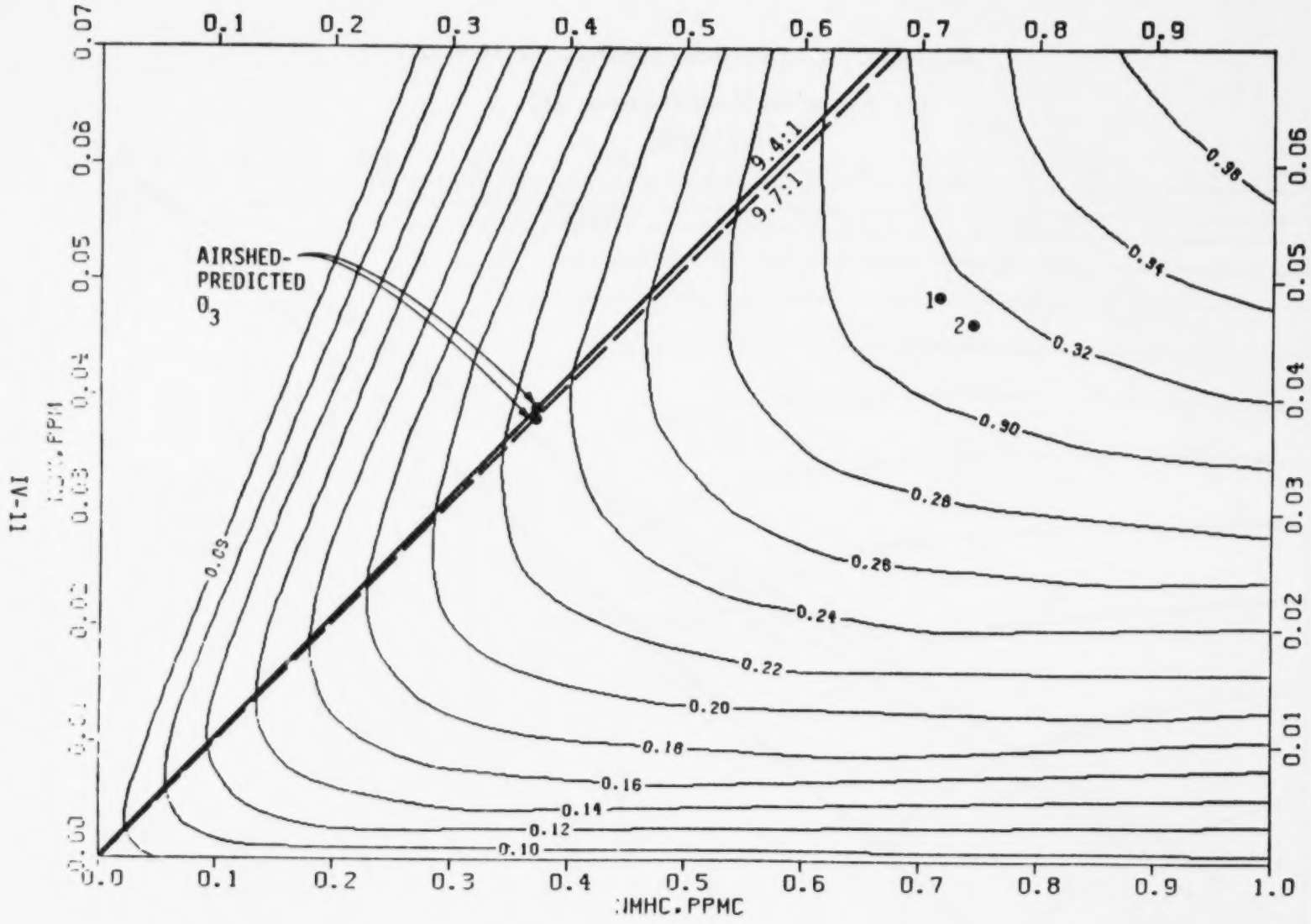
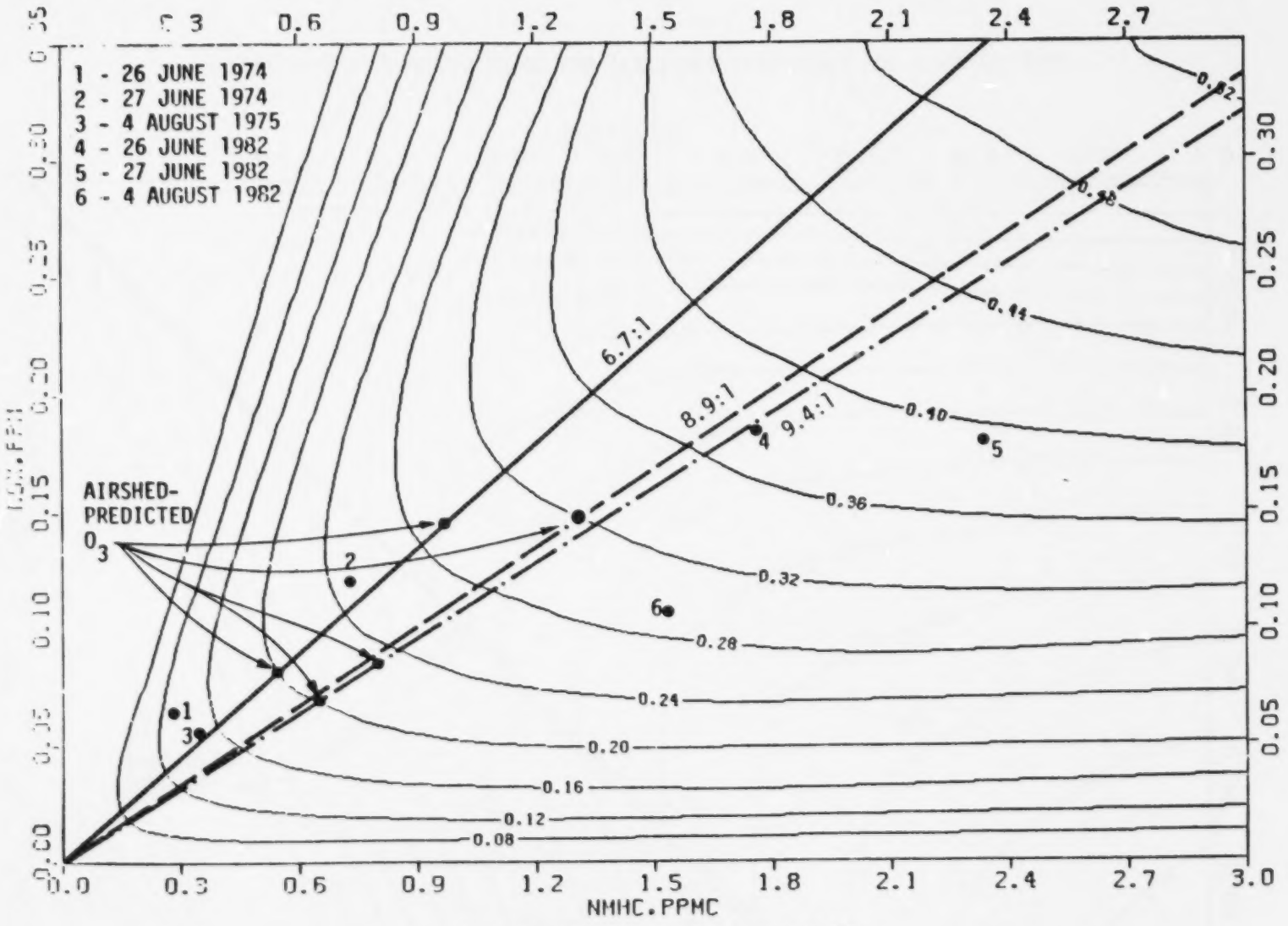
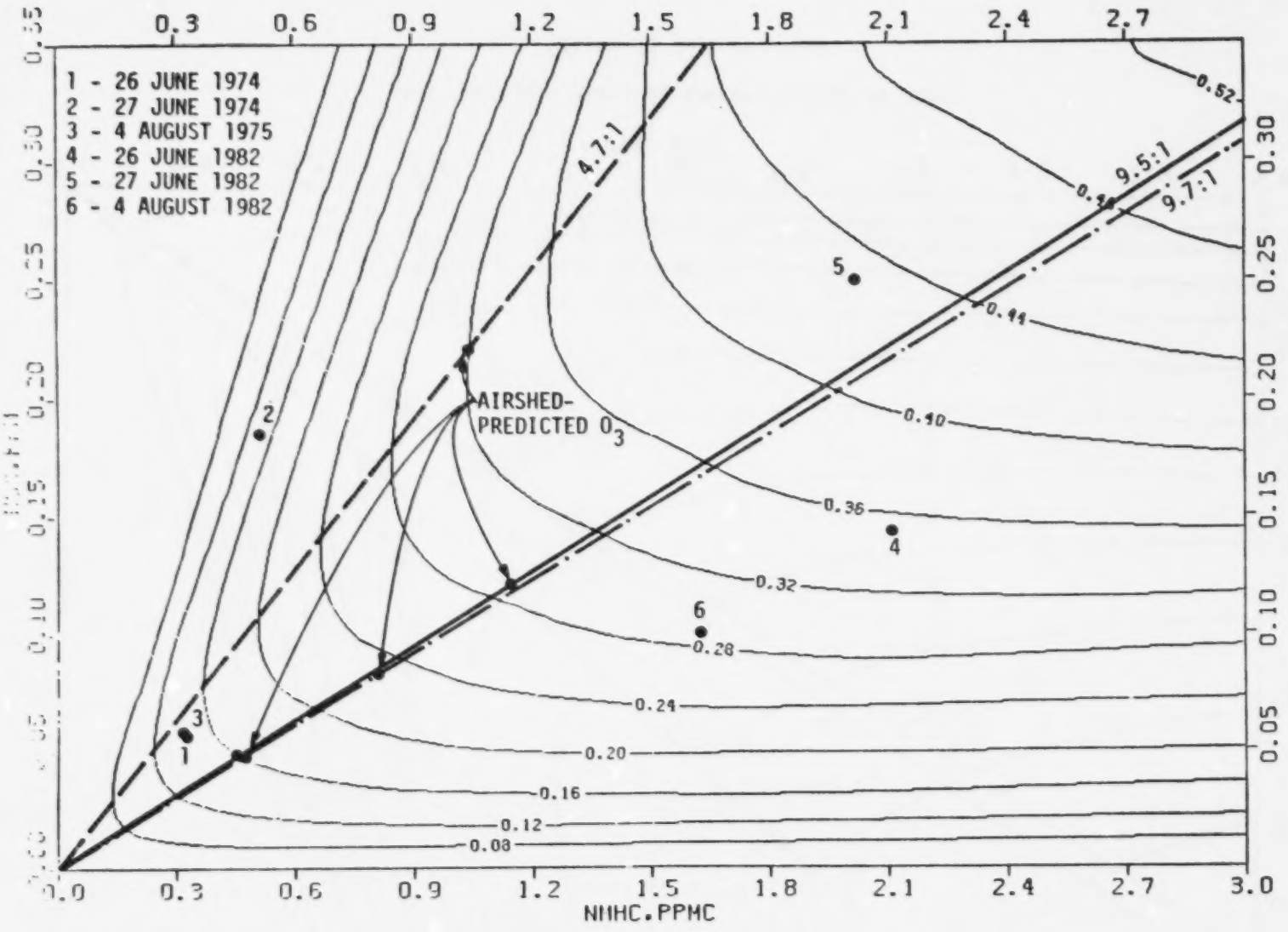


FIGURE IV-6. STANDARD OZIPP RUN (CITY-SPECIFIC EKMA) FOR 4 AUGUST 1982



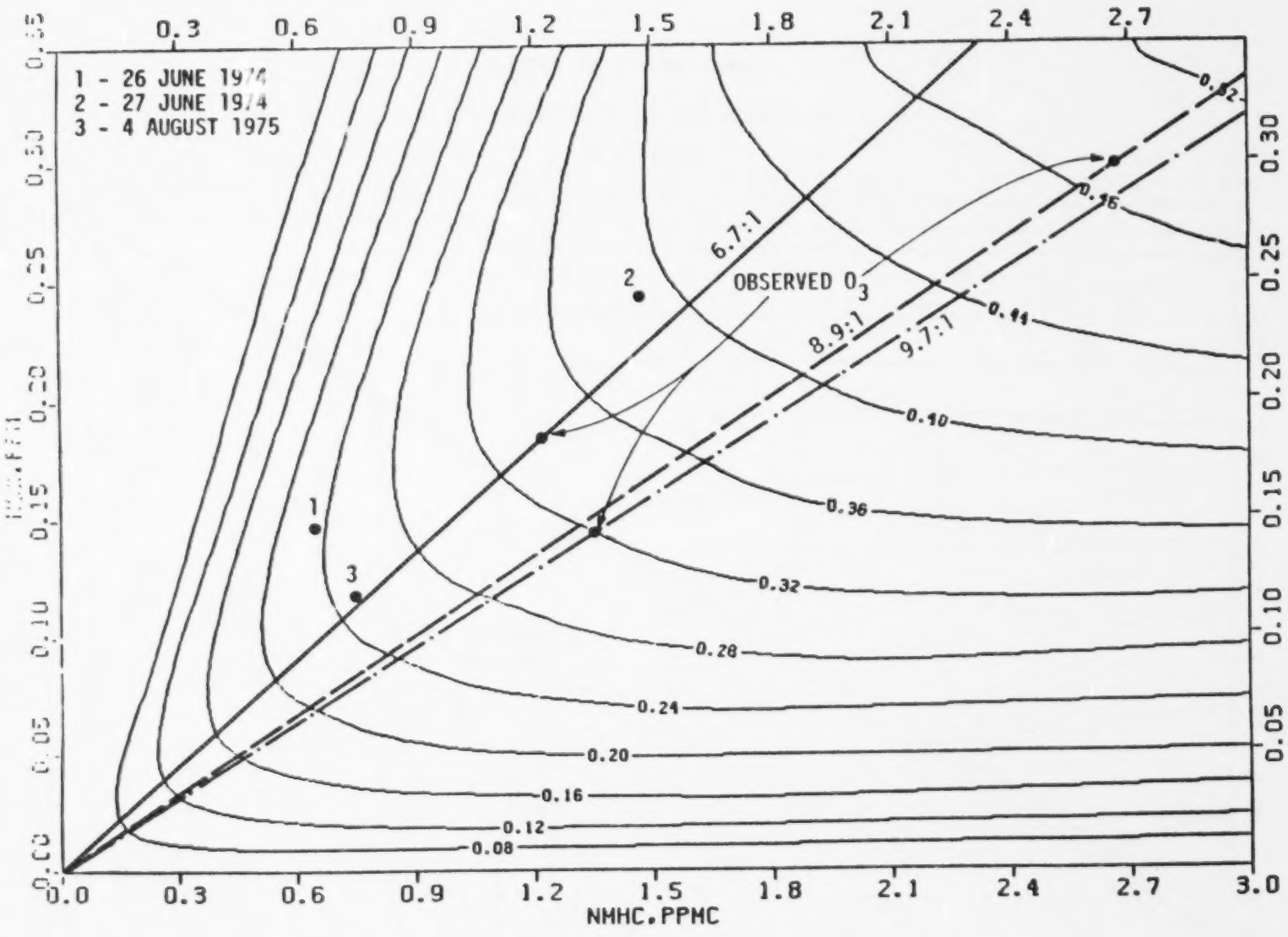
(a) Predictions using method (1)

FIGURE IV-7. STANDARD OZONE ISOPLETH CONDITIONS



(b) Predictions using method (2)

FIGURE IV-7 (Continued)



(c) Controls based on the prediction method

FIGURE IV-7 (Concluded)

Method 1 indicates how EKMA performance might compare with that of the Airshed Model if generalized (i.e., area-wide) controls were called for with EKMA, but in practice the controls were not distributed evenly. The "generalized" control was derived by comparing the total gridded emissions inventories for the region used by the Airshed Model in the base case and 1982 simulations. To calibrate EKMA to the Airshed Model, the design O_3 was taken from the highest O_3 simulated in the Airshed Model (at a monitoring site), and the HC/NO_x ratio was derived from averaging the simulated airshed precursor ratios from 0600 to 0900 PDT at the downtown Los Angeles monitoring site. Figures IV-1 through IV-6 illustrate the design O_3 values as AIRSHED-PREDICTED O_3; the HC/NO_x ratios are represented by a solid line in each figure; and the results of applying this method are shown as the points labeled 1. Each of the six figures (IV-I through IV-6) represents a trajectory-specific isopleth based on the city-specific calculations described in section III. Figure IV-7a (Level IV EKMA) shows the same set of design O_3 values and HC/NO_x ratio lines as figures IV-1 through IV-6, but the results for the six specific trajectories are labeled 1 through 6 in figure IV-7. All the design O_3 and relevant HC/NO_x ratios are also presented in table IV-2. The EKMA isopleth results are compared with the Airshed Model predictions in table IV-3.

Method 2 shows how the EKMA might perform compared with Airshed Model predictions when trajectory-specific emissions changes are applied. To calibrate the EKMA to the Airshed Model, the design O_3 values used in method 1 are used, but the HC/NO_x ratios are derived from the 0600 to 0900 PDT average HC and NO_x concentrations found in the SAI Trajectory Model simulations. The HC/NO_x ratios represent a trajectory-specific ratio that may be very different from the HC/NO_x ratios defined in method 1. The HC/NO_x ratios are shown in figures IV-1 to IV-7 as a dashed line. The results from applying method 2 are shown as points labeled 2 in figures IV-1 to IV-6. Figure IV-7(b) shows the same O_3 design values and HC/NO_x ratios used in method 2 on a Level IV EKMA and the results from all six emissions changes.

Method 3 (prediction method) shows the EKMA predictions using design O_3 values from monitoring station observations. To apply this method, we used the design HC/NO_x ratios from method 1 together with the total area emission changes. Design O_3 values are shown in figures IV-1 to IV-3 as OBSERVED O_3 on the HC/NO_x ratio (represented by a solid line). Results from applying the total area emission changes are shown as points labeled PREDICTED O_3 in figures IV-1 to IV-3. Figure IV-7(c) shows the prediction method results for the three days.

The results obtained with this set of isopleth diagrams can be presented in several ways. Previous model comparisons involved steps in a

TABLE IV-2. DESIGN O_3 AND HC/NO_x RATIOS USED IN THE EKMA PREDICTIONS

(a) Method (1):

> Total area emission changes
> Downtown Los Angeles 6:00 to 9:00 a.m. HC/NO_x from Airshed Model
> Design O_3 from Airshed Model

Date	Design O_3	HC/NO_x
26 June 1974	0.20	6.69
27 June 1974	0.32	8.92
4 August 1975	0.20	9.39
26 June 1982	0.29	6.69
27 June 1982	0.32	8.92
4 August 1982	0.23	9.39

(b) Method (2):

> Trajectory-specific emission changes
> Trajectory-specific 6:00 to 9:00 a.m. HC/NO_x
> Design O_3 from Airshed Model

Date	Design O_3	HC/NO_x
26 June 1974	0.20	9.52
27 June 1974	0.32	4.72
4 August 1975	0.20	9.72
26 June 1982	0.29	9.52
27 June 1982	0.32	4.72
4 August 1982	0.23	9.72

(c) Prediction Method:

> Total area emission changes
> Downtown Los Angeles 6:00 to 9:00 a.m. HC/NO_x from Airshed Model
> Observed design O_3

Date	Design O_3	HC/NO_x
26 June 1974	0.34	6.69
27 June 1974	0.49	8.92
4 August 1975	0.32	9.39

TABLE IV-3. COMPARISON OF OZONE PREDICTIONS FOR THE CITY-SPECIFIC EKMA, THE STANDARD-CONDITIONS (LEVEL IV) EKMA, AND THE SAI AIRSHED MODEL

(a) Method (1):

> Total area emission changes
> Downtown Los Angeles 6:00 to 9:00 a.m. HC/NO_x from Airshed Model
> Design O_3 from Airshed Model

Date	City-Specific EKMA	ΔO_3*	Level IV EKMA	ΔO_3*	Airshed Model: Over Whole Region	Airshed Model: Along Specific Trajectory
26 June 1974	0.12	-40	0.13	-35	0.29	0.13
27 June 1974	0.24	-25	0.25	-22	0.32	0.27
4 August 1975	0.14	-30	0.15	-25	0.23	0.11
26 June 1982	0.39	+35	0.37	+28	0.20	0.31
27 June 1982	0.42	+31	0.39	+22	0.32	0.25
4 August 1982	0.31	+35	0.29	+26	0.20	0.24

(b) Method (2):

> Trajectory-specific emission changes
> Trajectory-specific 6:00 to 9:00 a.m. HC/NO_x
> Design O_3 from Airshed Model

Date	City-Specific EKMA	ΔO_3*	Level IV EKMA	ΔO_3*	Airshed Model: Over Whole Region	Airshed Model: Along Specific Trajectory
26 June 1974	0.14	-30	0.14	-30	0.29	0.13
27 June 1974	0.14	-56	0.14	-56	0.32	0.27
4 August 1975	0.14	-30	0.14	-30	0.23	0.11
26 June 1982	0.35	+21	0.35	+21	0.20	0.31
27 June 1982	--	--	0.43	+34	0.32	0.25
4 August 1982	0.31	+35	0.29	+26	0.20	0.24

TABLE IV-3 (Concluded)

(c) Prediction Method:

> Total area emission changes
> Downtown Los Angeles 6:00 to 9:00 a.m. HC/NO_x from Airshed Model
> Observed design O_3

Date	City-Specific EKMA	ΔO_3*	Level IV EKMA	ΔO_3*
26 June 1974	0.19	-44	0.24	-29
27 June 1974	0.36	-27	0.39	-20
4 August 1975	0.22	-31	0.25	-22

* Percentage change in ozone = $\frac{(\text{Predicted } O_3) - (\text{Design } O_3)}{(\text{Design } O_3)} \times 100$

series; the isopleth approach allows a "recalibration" back to the point on which one wishes to base the relative comparison. On the other hand, the predictions of the more sophisticated models involve changes in reactivity, diurnal emission patterns, and even the trajectory path itself, which predictions based on single isopleth diagrams cannot simulate.

The three methods of comparison shown in table IV-2 are based on the values of maximum ozone concentrations found in the SAI airshed simulations. For the base case days (1974 and 1975) we used the maximum ozone concentrations found in the SAI airshed simulations at the monitoring sites (station maximum ozone). For the future-year days (1982) we used the maximum ozone concentration found anywhere in the modeling region (regional maximum ozone) in the SAI airshed simulations. Often the regional maximum ozone value is greater than the maximum ozone value at the station due to the continuation of the chemistry and transport. This is especially true when station maximum ozone observations occur early in the afternoon. Thus, the design O_3 values for 1982 shown in table IV-2 are higher than those for 1974 and 1975.

The Airshed Model "predictions" included in table IV-3 are repeated from table III-1; for the changes across the entire modeling region, the Airshed Model numbers are actually the transposed design O_3 values found in table IV-2. The results presented in table IV-3 show that on a relative basis the EKMA tends to be more sensitive to emission changes than the Airshed Model over the entire basin, even though the changes predicted along specific trajectories are similar. A perplexing exception to this similarity is seen in the method (2) comparison based on the 27 June 1974 trajectory. For this case the design HC/NO_x and emissions changes were made for the specific trajectory; however, agreement with the Airshed Model was much better when basin-wide emissions and the downtown HC/NO_x ratio were used. The 27 June 1982 trajectory-specific comparison [method (2)] disclosed another problem; the specific HC/NO_x ratio of 4.72 was so low that the design ozone level could never be reached. A similar situation was reported by Feldstein et al. (1979) for the San Francisco area.

The second type of comparison involves the use of EKMA diagrams to predict future observations based on past observations. In this case, comparison of the SAI grid and trajectory models is not as appropriate since these models are not "calibrated" to past observations. For this comparison, the model series is used and the predictions of the various EKMA type models are of interest. The Airshed Model base case HC/NO_x ratios were used for the city-specific and Level IV predictions shown on the isopleth diagrams by PREDICTED O_3. These HC/NO_x ratios were used because the observed ratios have been a subject of controversy and have

changed because of recalibration. The ratios generated by the emission inventory in the grid model for the downtown area provide a self-consistent reference across the model series for this study. These relative predictions, based on observations, are shown in table IV-3, which is similar to table III-1 showing the absolute predictions.

In the third method of comparison, the base case ozone values and the HC/NO_x ratios for the city-specific and Level IV predictions were taken from the absolute prediction study. Thus, the predictions were based on the 0800 PDT HC and NO_x values generated by the more sophisticated model in the series, namely, the model with a modified mixing-height algorithm started at 0500 PDT hours. Since both the city-specific and Level IV models start at 0800, the initial HC/NO_x values are the same. These predictions are also shown in table IV-4; the predictions are shown graphically on the isopleth diagrams by (3) in figures IV-8 through IV-10 for the city-specific case and figure IV-11 for the standard Level IV diagram. This relative prediction comparison is discussed next with the presentation of the modified isopleths. Table IV-4 shows that the city-specific EKMA and Level IV EKMA models predict identical concentrations for 1982 using the 1974 trajectories; however the city-specific EKMA tends to predict lower ozone concentrations for 1982 than the Level IV EKMA when the 4 August 1975 trajectory is used.

B. A NEW TYPE OF ISOPLETH DIAGRAM

In the past, the EKMA has used an isopleth diagram based on initial concentrations of HC and NO_x during the period from 6:00 to 9:00 a.m., more specifically, those at 0800 hours. When the regular EKMA isopleth diagrams are used to estimate changes in maximum ozone concentrations resulting from changes in HC and NO_x emissions, the observed 6:00 to 9:00 a.m. HC/NO_x ratio is used with the maximum observed ozone concentration to locate a starting point on the isopleth diagram. Relative changes in the HC and NO_x values making up the ordinate and abscissa of the isopleth diagram are equated to relative changes in emissions to find the predicted ozone value. Alternatively, the relative changes in the HC and NO_x values necessary to reach some desired ozone value are equated to the necessary relative changes in emissions.

This section describes a new method of locating the starting point on a new isopleth diagram that is based on the relative emission inventories of HC and NO_x. There are several reasons for introducing a new type of isopleth diagram:

TABLE IV-4. A COMPARISON OF 1982 OZONE PREDICTIONS FOR THE ISOPLETH MODELS (OZONE CONCENTRATIONS IN PPM)

Date	SAI Trajectory	CBM-EKMA	EKMA IIa	City-Specific EKMA	Level IV EKMA
26 June 1974					
design O_3 = 0.30	0.21	0.18	0.13	0.20	0.22
design O_3 = 0.19	--	--	0.11	0.14	0.14
design O_3 = 0.20	--	--	--	0.14	0.14
27 June 1974					
design O_3 = 0.32	0.29	0.17	0.19	0.20	0.22
design O_3 = 0.30	--	0.18	0.19	0.20	0.20
design O_3 = 0.21	--	--	0.13	0.14	0.14
4 August 1975					
design O_3 = 0.34	0.22	0.22	0.23	0.23	0.26
design O_3 = 0.35	--	0.21	0.24	0.24	0.26
design O_3 = 0.26	--	--	0.18	0.17	0.20
design O_3 = 0.28	--	--	--	0.21	0.21

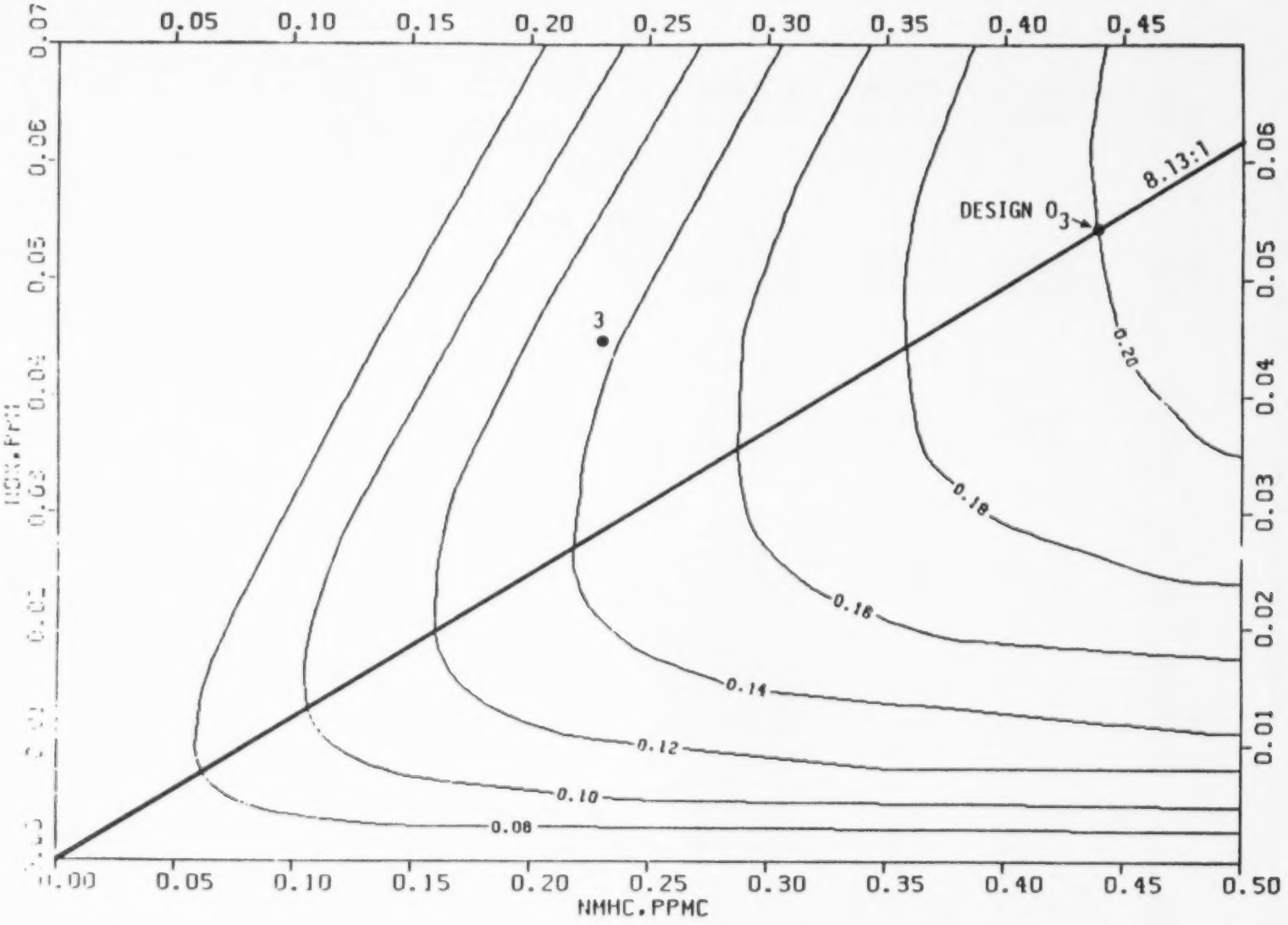


FIGURE IV-8. STANDARD OZIPP RUN (CITY-SPECIFIC EKMA) FOR 26 JUNE 1974: METHOD (3)

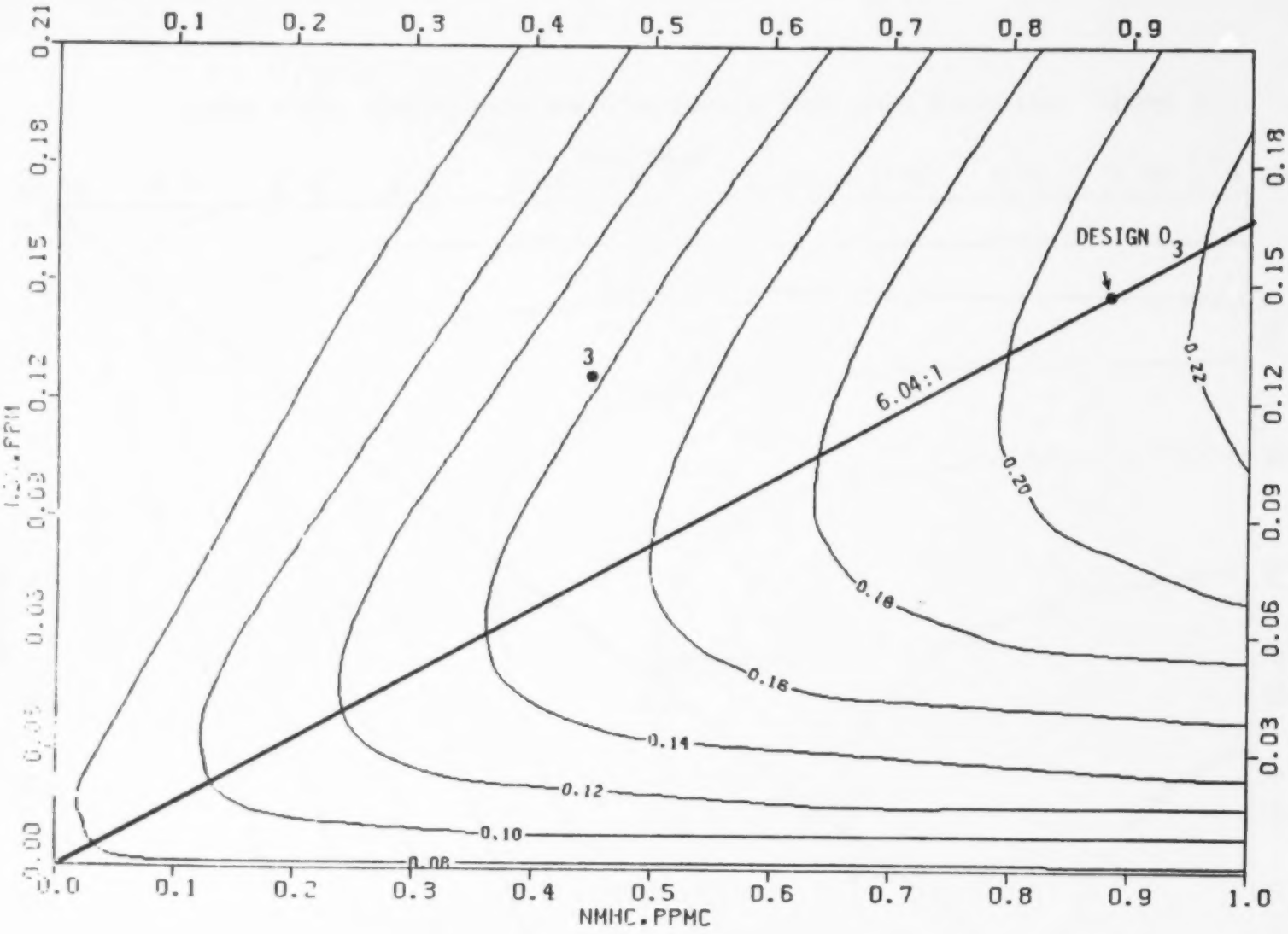


FIGURE IV-9. STANDARD OZIPP RUN (CITY-SPECIFIC EKMA) FOR 27 JUNE 1974: METHOD (3)

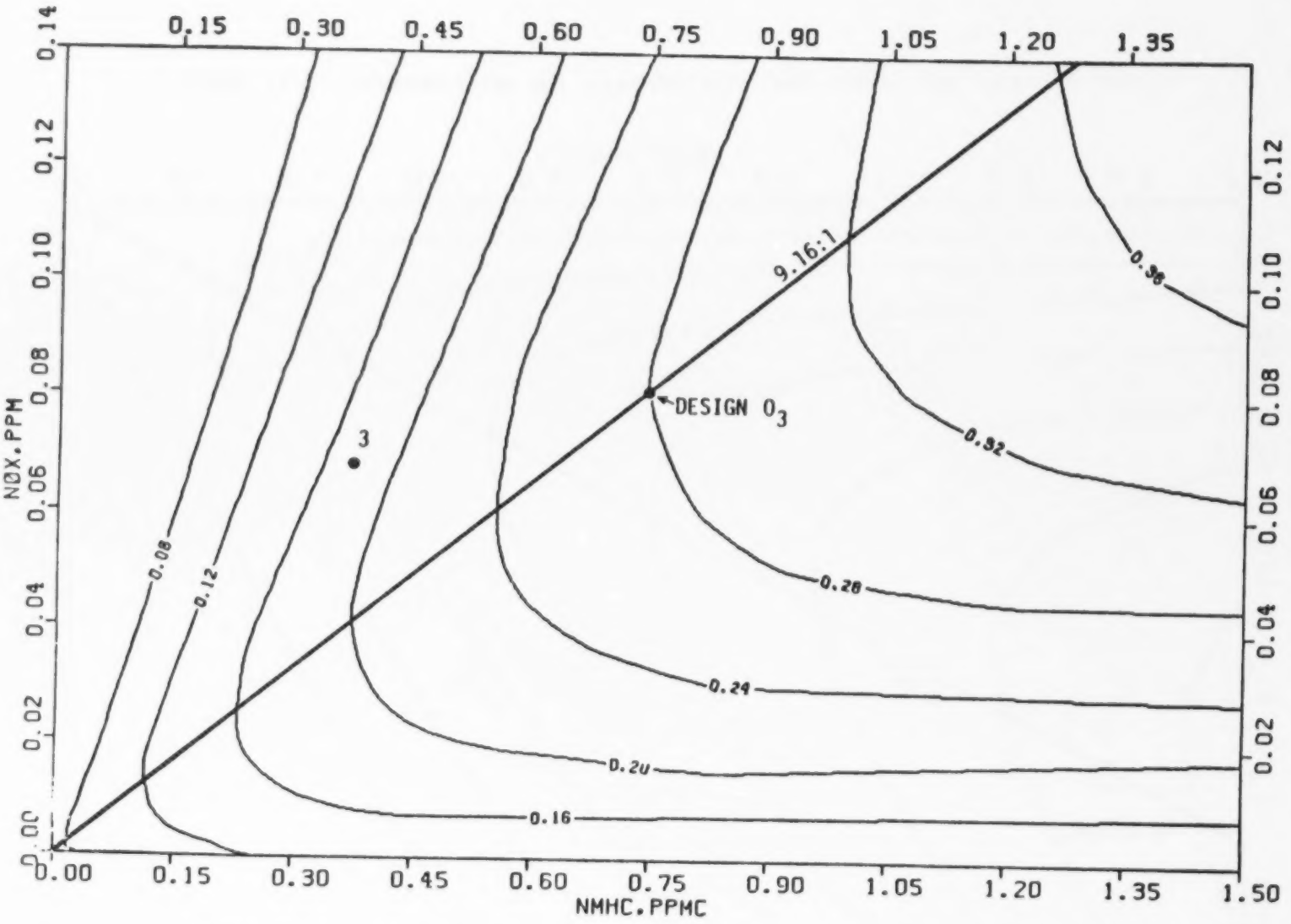


FIGURE IV-10. STANDARD OZIPP RUN (CITY-SPECIFIC EKMA) FOR 4 AUGUST 1975: METHOD (3)

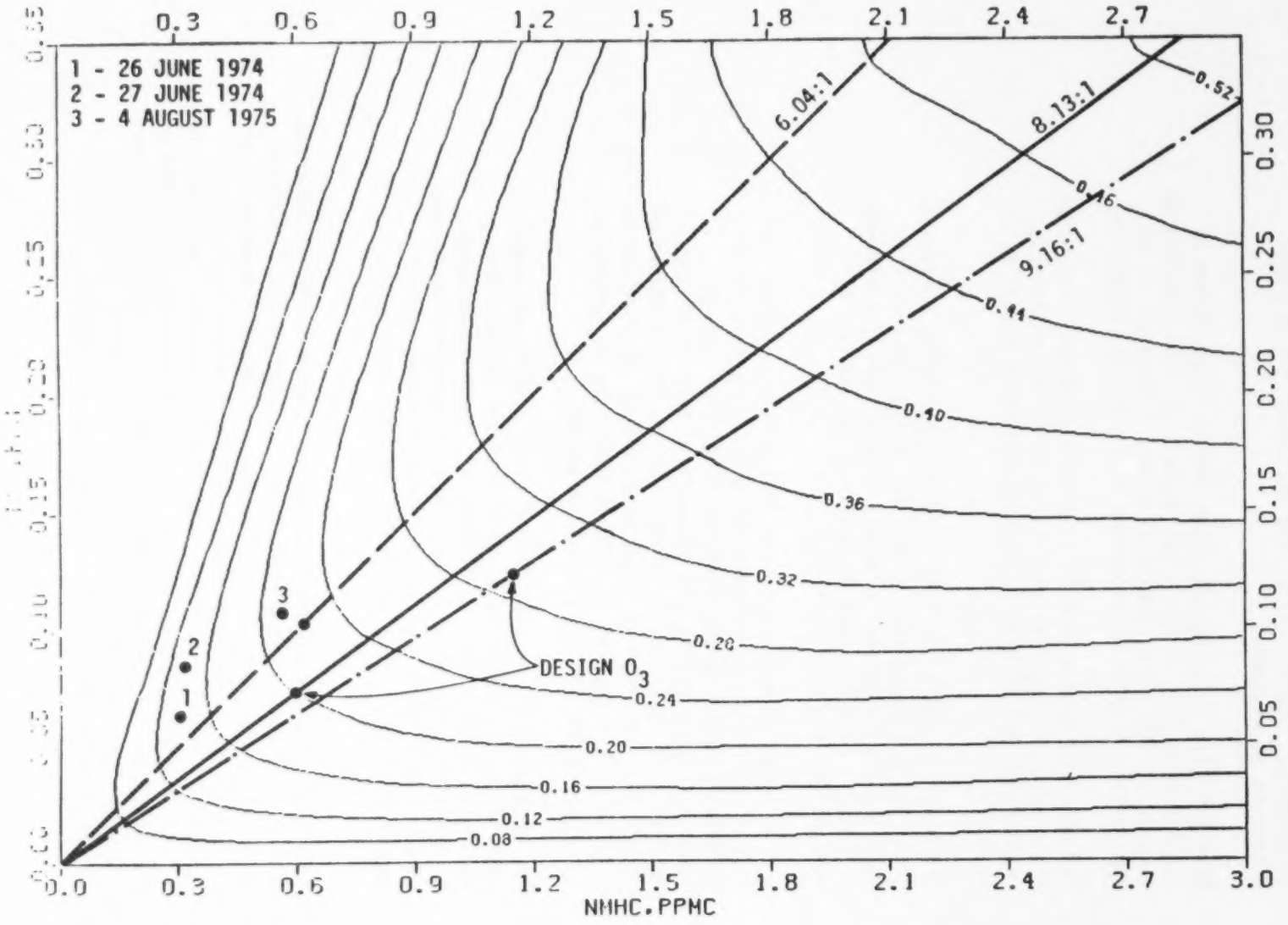


FIGURE IV-11. STANDARD OZONE ISOPLETH CONDITIONS: METHOD (3) EMISSION CHANGES

- The ambient HC/NO_x ratio is often difficult to measure accurately. (Specifically, the HC values are the most difficult to measure.)

- Even accurate measurements often show a large degree of scatter from hour to hour, day to day, or from location to location, within the same urban area. Expression of an appropriate average thus becomes difficult and uncertain.

- The observed ratios of 6:00 to 9:00 a.m. HC/NO_x concentrations rarely agree with the ratios of HC/NO_x emissions, even though the morning precursors should be essentially unreacted.

- The observed ratios of 6:00 to 9:00 a.m. HC/NO_x concentrations may not agree with simulated ratios found in very sophisticated atmospheric models. This lack of agreement is rarely, if ever, used to evaluate the quality or appropriateness of such models.

- It has never been demonstrated that relative changes in 6:00 to 9:00 a.m. concentrations are a good measure of relative changes in the emission inventory. On the contrary, the opposite was shown to be true by Whitten, Meldgin, and Roth (1977). They reported that a simulated 24 percent reduction in total emissions of HC resulted in a 41 percent reduction in 6:00 to 9:00 a.m. HC concentrations using the SAI grid model in Denver.

- The present EKMA diagrams do not always relate to a base case trajectory model simulation that can be used to validate, or gain some indication of, model performance. If the EKMA trajectory is dominated by post-0800 emissions of an HC/NO_x ratio that is different from the initial condition values, then validation is very difficult.

Thus the main feature of the new type of diagram is the elimination of the 6:00 to 9:00 a.m. HC/NO_x dependence. The ordinate and abscissa become the relative emissions of NO_x and HC. To suppress dependence on the initial conditions, the model starting time is moved sufficiently forward so that the local emissions significantly dominate the production of ozone. The justification for an early starting time was given earlier in the discussion of the CBM-EKMA trajectory model. Initial conditions are treated only as transported pollutants in the surface layer. The following list details specific features of the new method:

- Ambient HC and NO_x measurements are not required. However, any such available data can be used to validate or provide some measure of performance for the trajectory model using the base case emissions inventory, which defines the (1,1) point of the isopleth diagram.

- Emission inventories, which are required for the new method, are already required under Section 172.(b) for nonattainment areas.

- Since the scales of the ordinate and abscissa of the new diagrams are relative emissions, the predictions of the new EKMA method relate directly to changes in emissions. Dependence on initial concentrations is minimized, whereas dependence on those emissions that are to be controlled is maximized.

- The line from the origin through the (1,1) point using the new method becomes the equivalent line to the HC/NO_x ratio line in the original EKMA. That is, the design or staring point ozone is located along this line. However, this line has a new feature not readily apparent in a comparison with the original EKMA. The distance between the (1,1) point and the observed ozone is an instant and clear measure of performance. Except for an unequal bias of errors between the HC and NO_x inventories, the combined dispersion, chemistry, and inventory errors should lie along this line.

Examples of the new type of isopleth diagram are shown in figures IV-12 through IV-17 for the CBM-EKMA and figures IV-18 through IV-23 for the EKMA IIa model. The center of the diagram, the (1,1) point, corresponds to the CBM-EKMA trajectory model runs of table III-1 discussed earlier. The (2,2) point corresponds to a doubling of both HC and NO_x emissions. Initial concentrations and precursor concentrations aloft were rolled back (or up) linearly according to the location on the isopleth diagram. Ozone values aloft were adjusted by the following formula:

$$[O_3]_{aloft} = 0.04 + (HC + NO_x)/2 \quad ,$$

where HC and NO_x refer to the location on the isopleth diagram. The use of the isopleth diagram is similar to the original EKMA version except

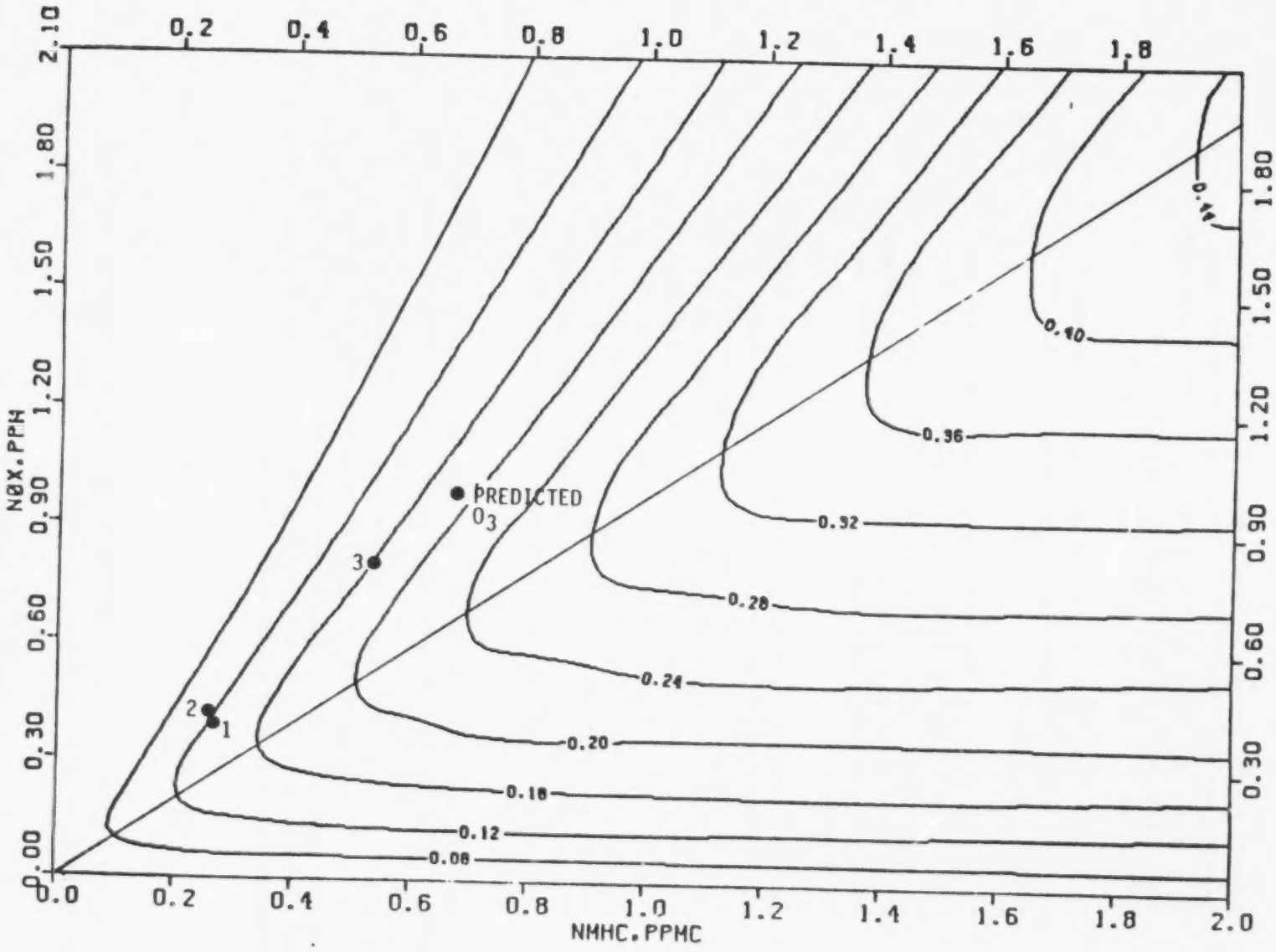


FIGURE IV-12. CBM-EKMA TRAJECTORY: 26 JUNE 1974--BASE CASE

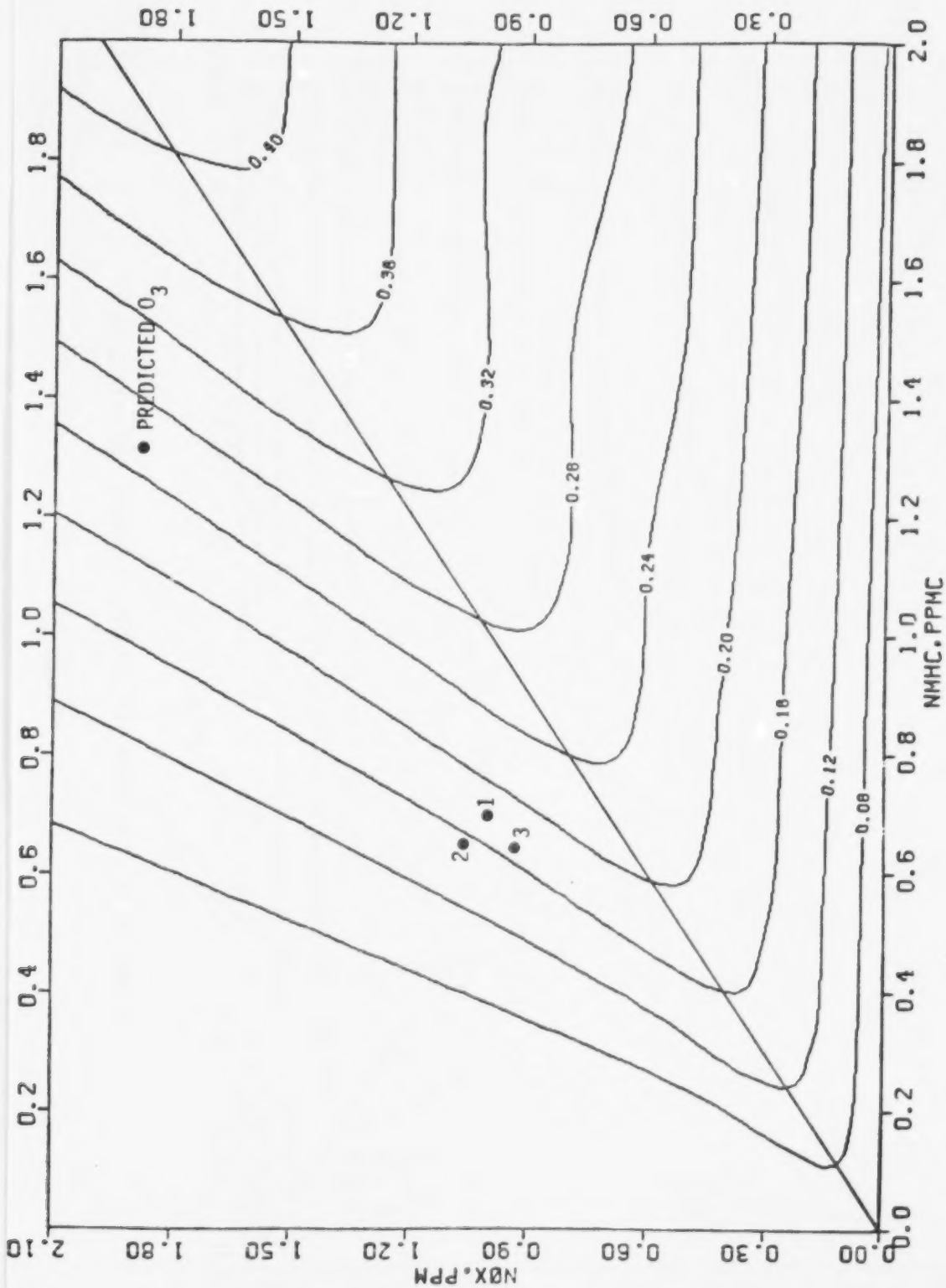


FIGURE IV-13. CBM-EKMA TRAJECTORY: 27 JUNE 1974--BASE CASE

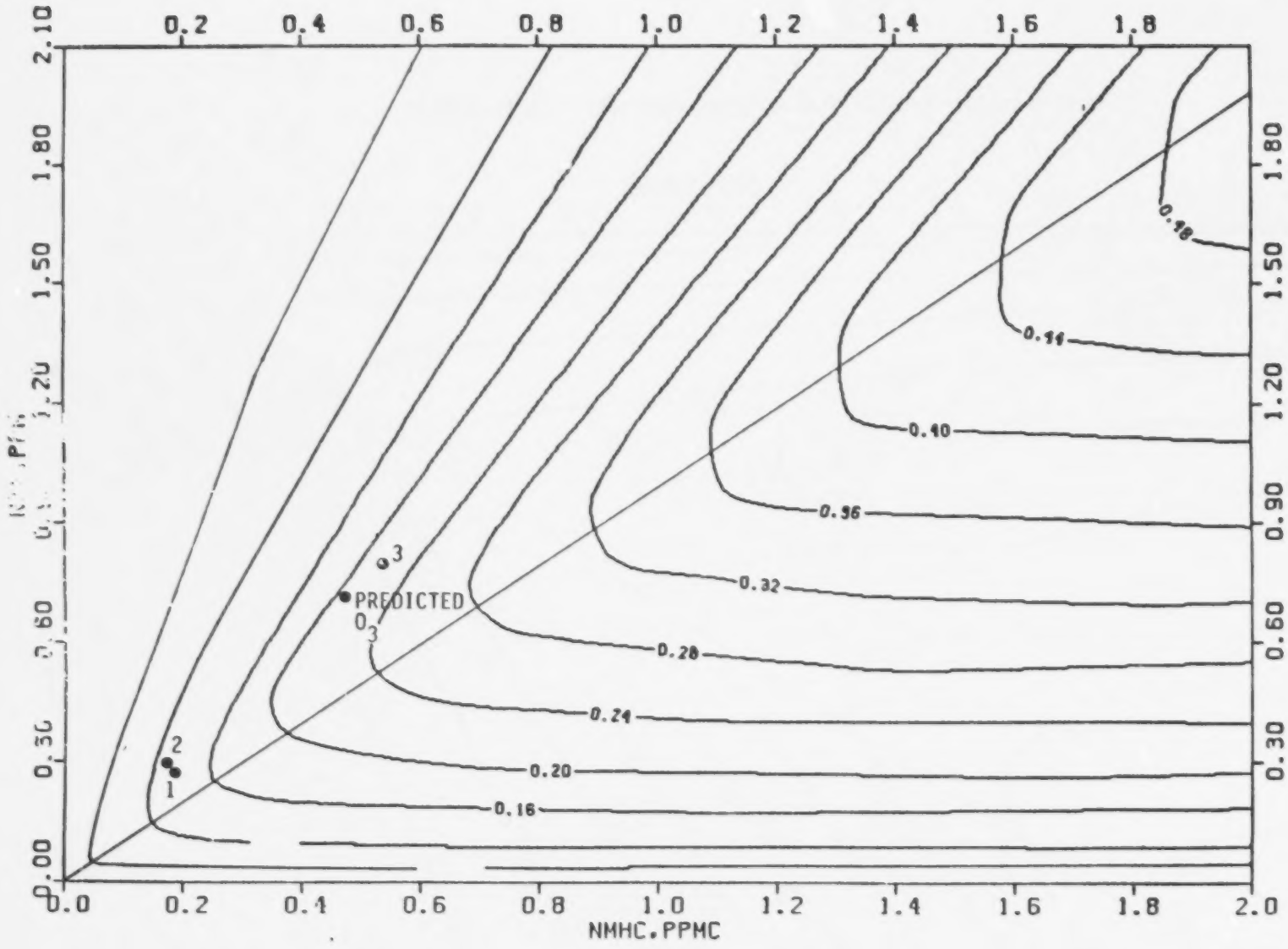


FIGURE IV-14. CBM-EKMA TRAJECTORY: 4 AUGUST 1975--BASE CASE

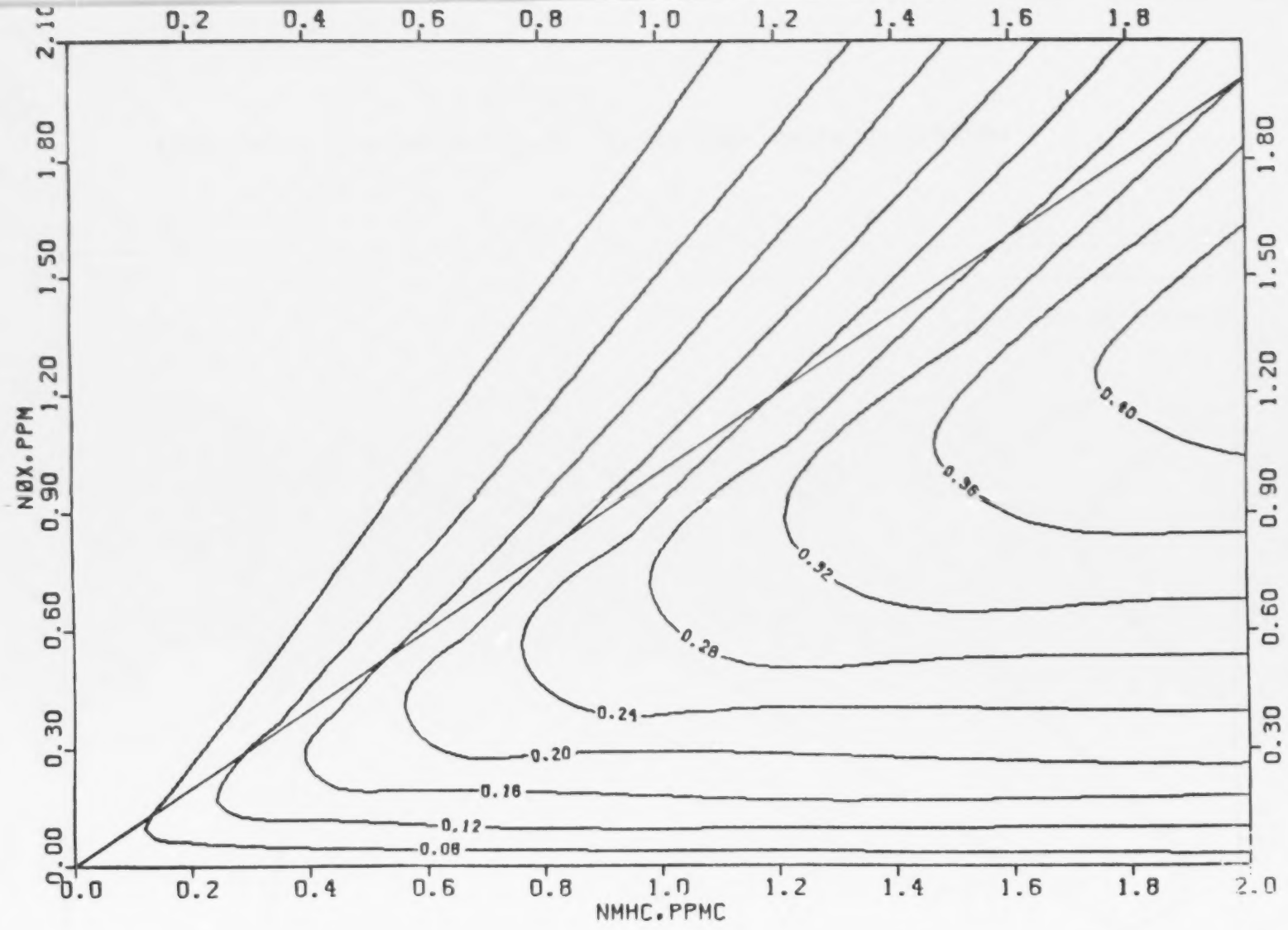


FIGURE IV-15. CBM-EKMA TRAJECTORY: 26 JUNE 1982--DIFFERENT TRAJECTORY

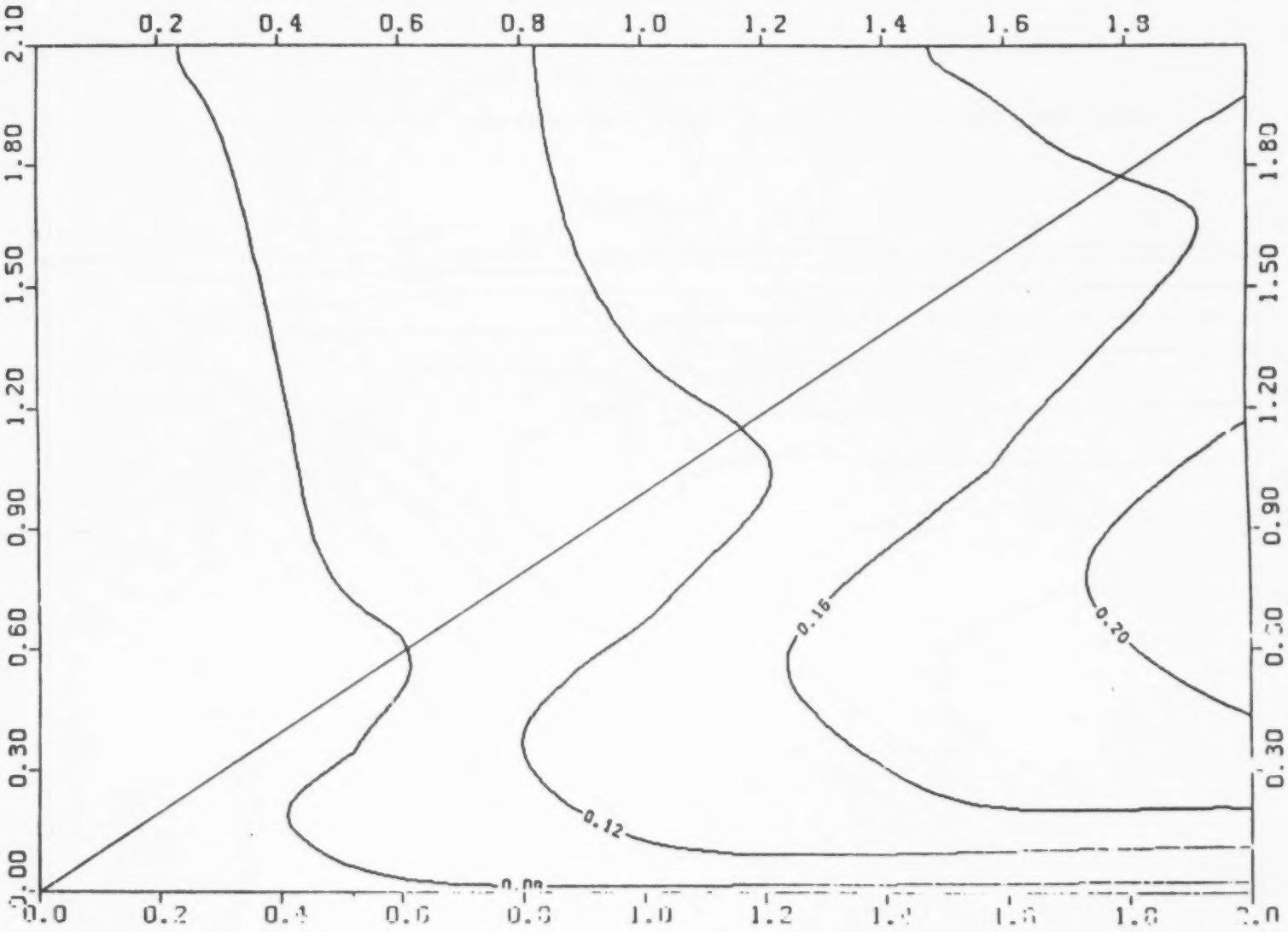


FIGURE IV-16. CBM-EKMA TRAJECTORY: 27 JUNE 1982--DIFFERENT TRAJECTORY

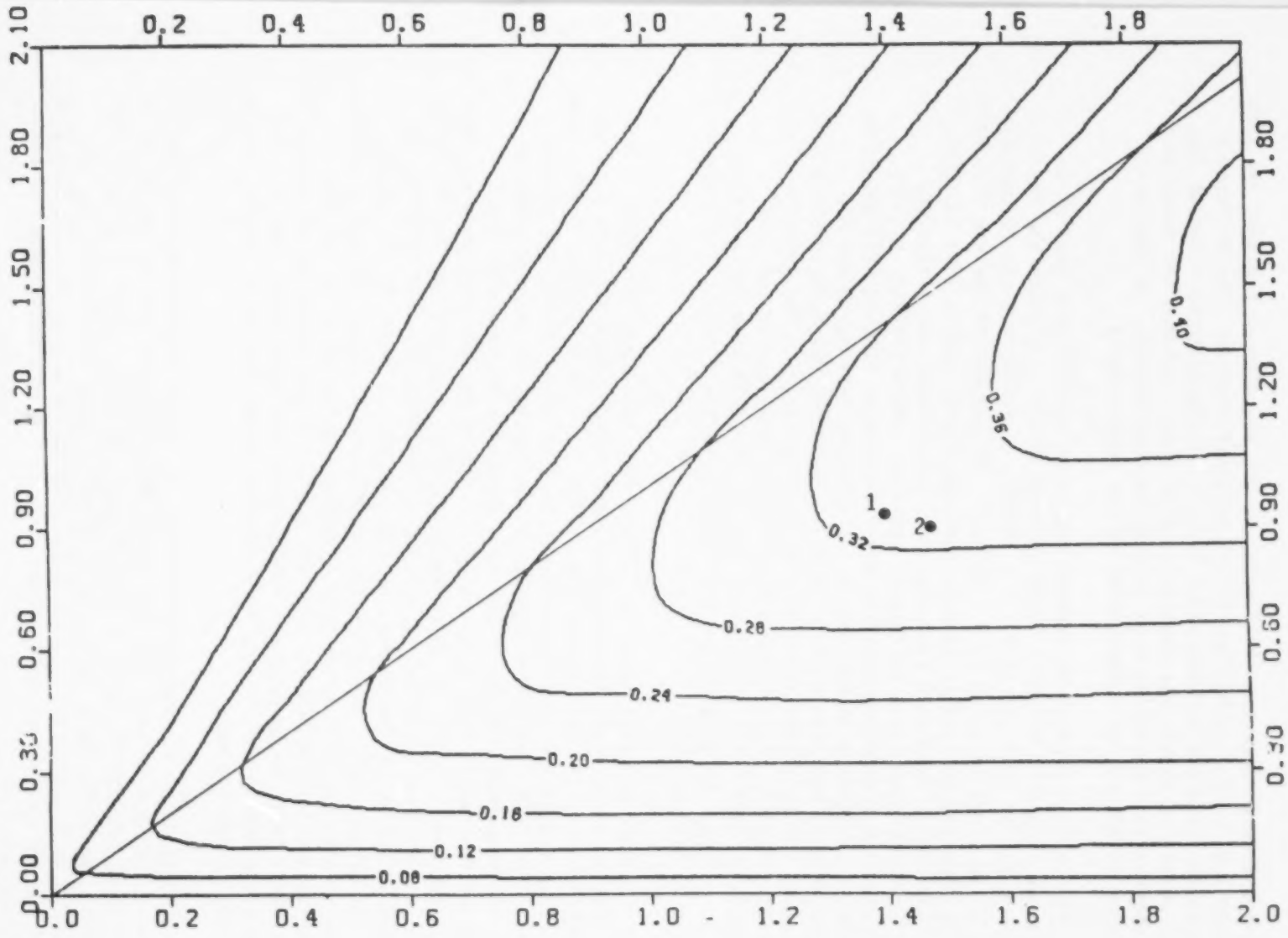


FIGURE IV-17. CBM-EKMA TRAJECTORY: 4 AUGUST 1982--DIFFERENT TRAJECTORY

that the line through the (1,1) point in the new diagram replaces the 6:00 to 9:00 a.m. HC/NO_x ratio line of the original diagram. The difference between the observed maximum ozone and the simulated ozone value at the (1,1) point represents the cumulative discrepancy between the model and the observations resulting from inaccurate measurements, an inaccurate emission inventory, or inadequacies of the model itself.

The various prediction methods discussed earlier were applied to these new isopleths (figures IV-18 through IV-23) to produce the results given in tables IV-4 and IV-5. The results in table IV-5 can be compared with those given in table IV-3. However, the changes in the new isopleths for transported pollutants tend to generate higher sensitivity to control than the normal isopleths (and the SAI Airshed Model and trajectory model), which keep these pollutants constant. Nevertheless, results obtained with trajectory-specific emission changes [method (2)] show the greatest sensitivity to the specific trajectory path using the new isopleths when compared with the normal isopleths, which all predict 0.14 ppm using the base case (1974 and 1975) trajectories. The CBM-EKMA predicts slightly lower ozone concentrations than any of the other versions of EKMA. The predictions for 27 June 1982 show the greatest variance among the models; the new isopleth versions show significantly less predicted ozone.

It should be noted that the 27 June 1982 base case isopleths in both the regular and new versions have a rather unusual general shape that was reported earlier by Whitten and Hogo (1978). In this report, it was shown that such shapes are caused by two maxima that occur during the simulations. The OZIPP and OZIPM codes pick the highest of the two peaks so that the resultant diagram is really a composite of two more normal diagrams that would plot only one peak. A more serious problem with some isopleths based on this 27 June 1982 trajectory involved the use of design ozone values that could not be located on the diagram. This problem was caused by the gross difference, originally seen in table III-1, between the SAI Airshed Model and trajectory model results (0.32 ppm and 0.12 ppm, respectively) for this trajectory. Hence, the "calibration" of the relative isopleth method was too severe when it was necessary to extend it to a model that, on an absolute scale, predicted much lower levels. The EKMA-style models all originally simulated rather low ozone levels, as did the SAI trajectory model.

The rollback of transported pollutants cannot totally explain the gross difference between the 1982 CBM-EKMA prediction and the SAI trajectory model prediction based on the 27 June 1974 data shown in a comparison of the results in table IV-4. As originally shown in table III-1, the CBM-EKMA used the specific trajectory information along the same 1974 path from the SAI trajectory model outputs using the 1982 emissions. In table

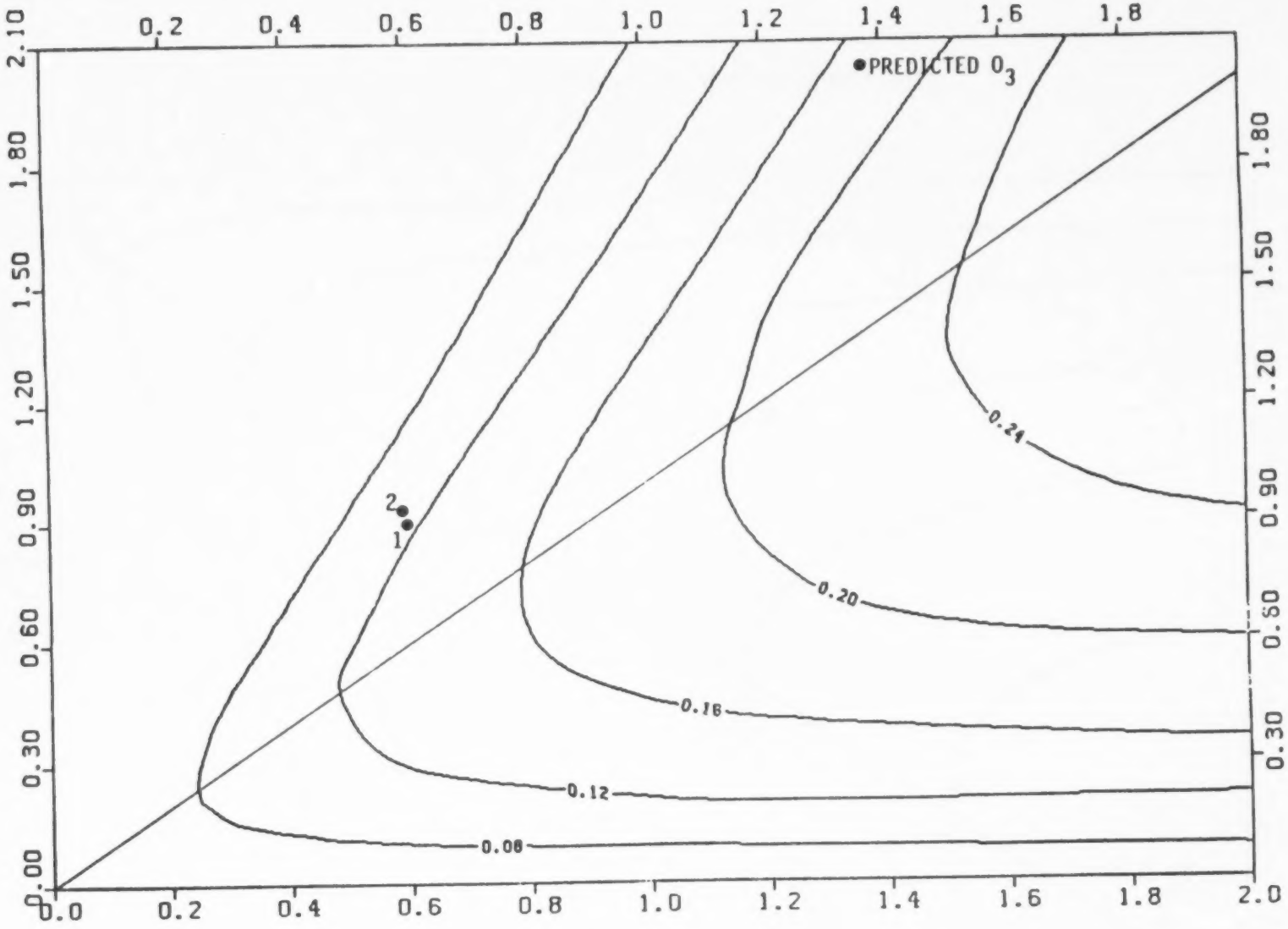


FIGURE IV-18. EKMA IIa TRAJECTORY: 26 JUNE 1974--BASE CASE

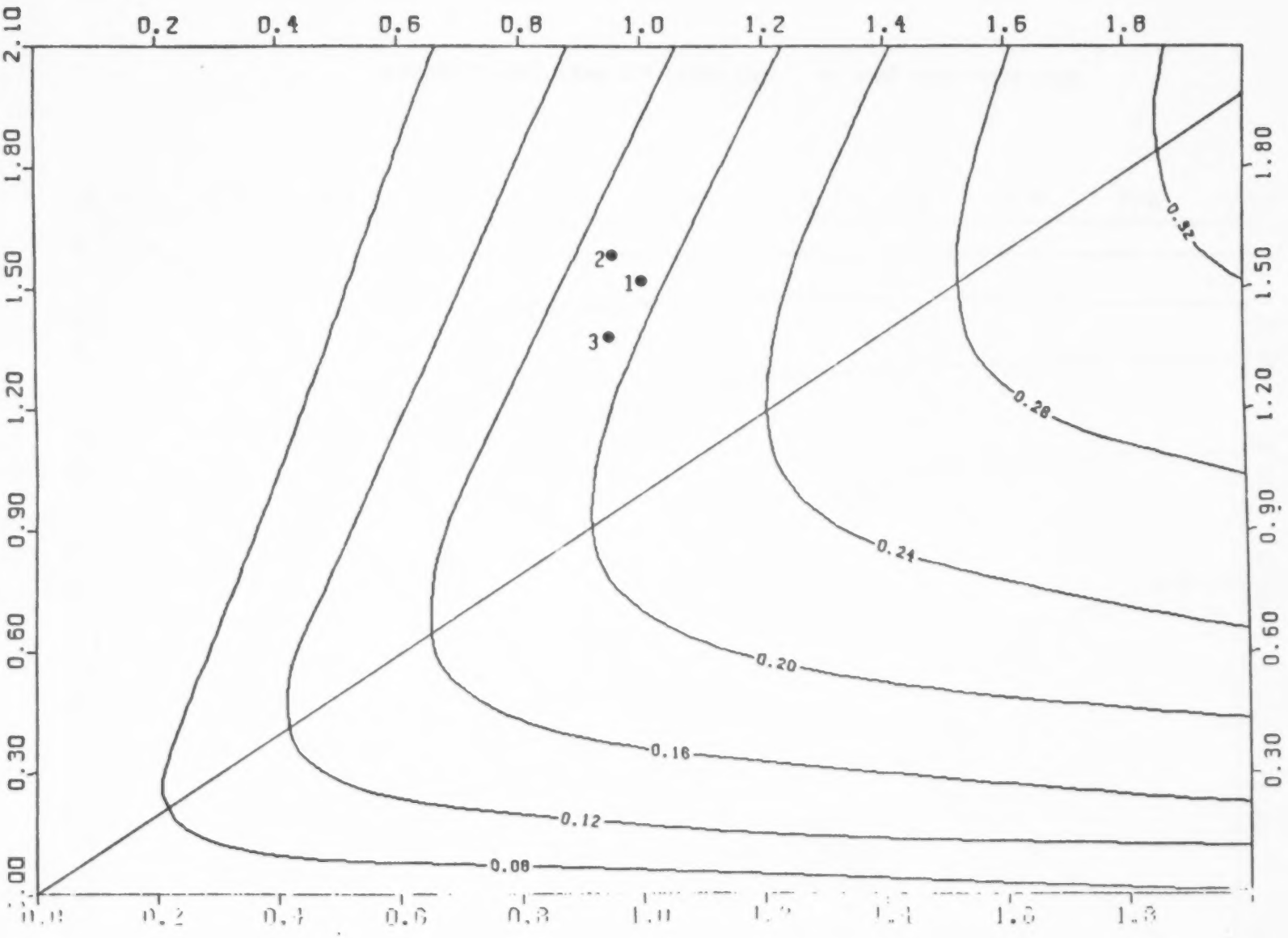


FIGURE IV-19. EKMA IIa TRAJECTORY: 27 JUNE 1974--BASE CASE

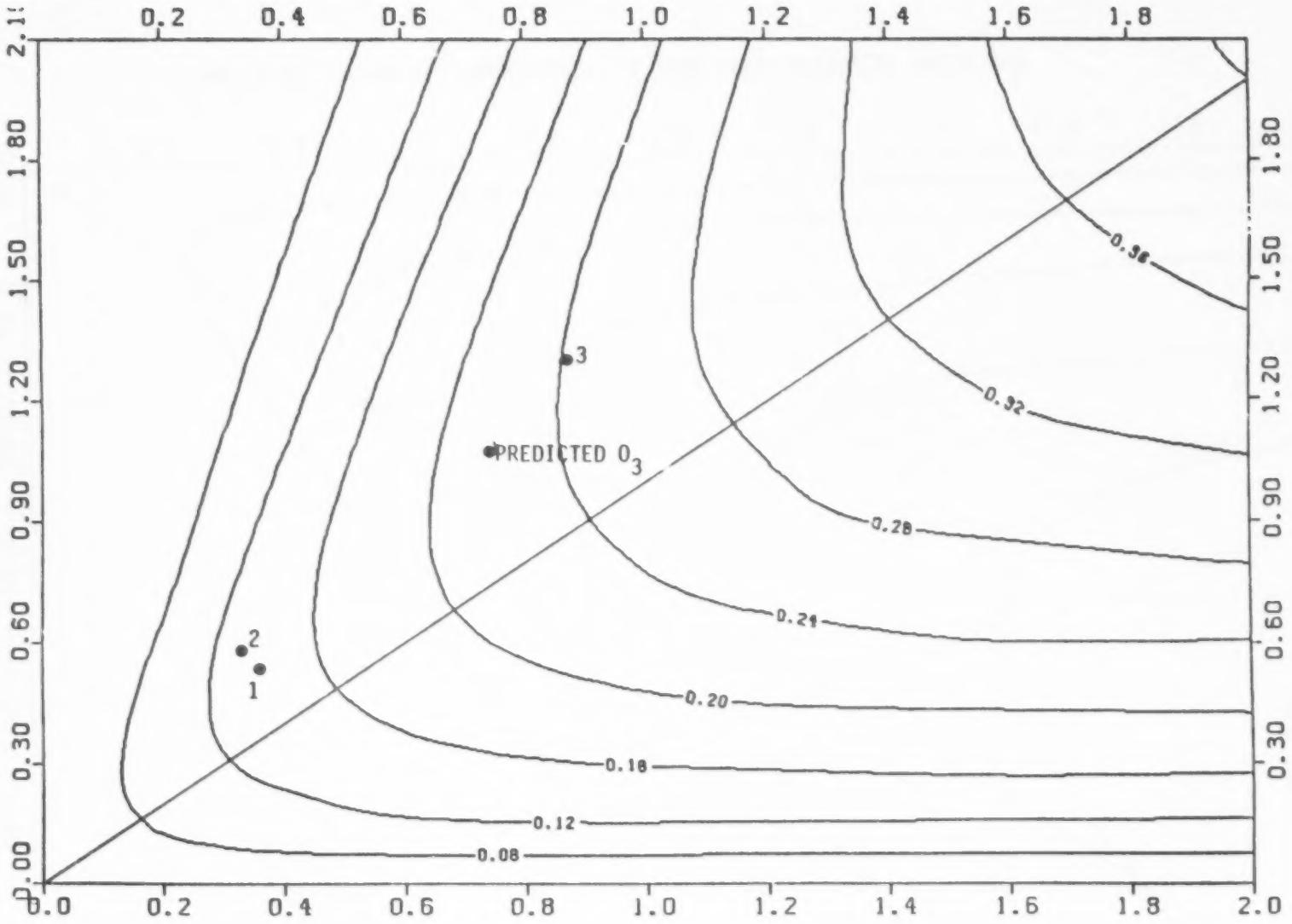


FIGURE IV-20. EKMA IIa TRAJECTORY: 4 AUGUST 1975--BASE CASE

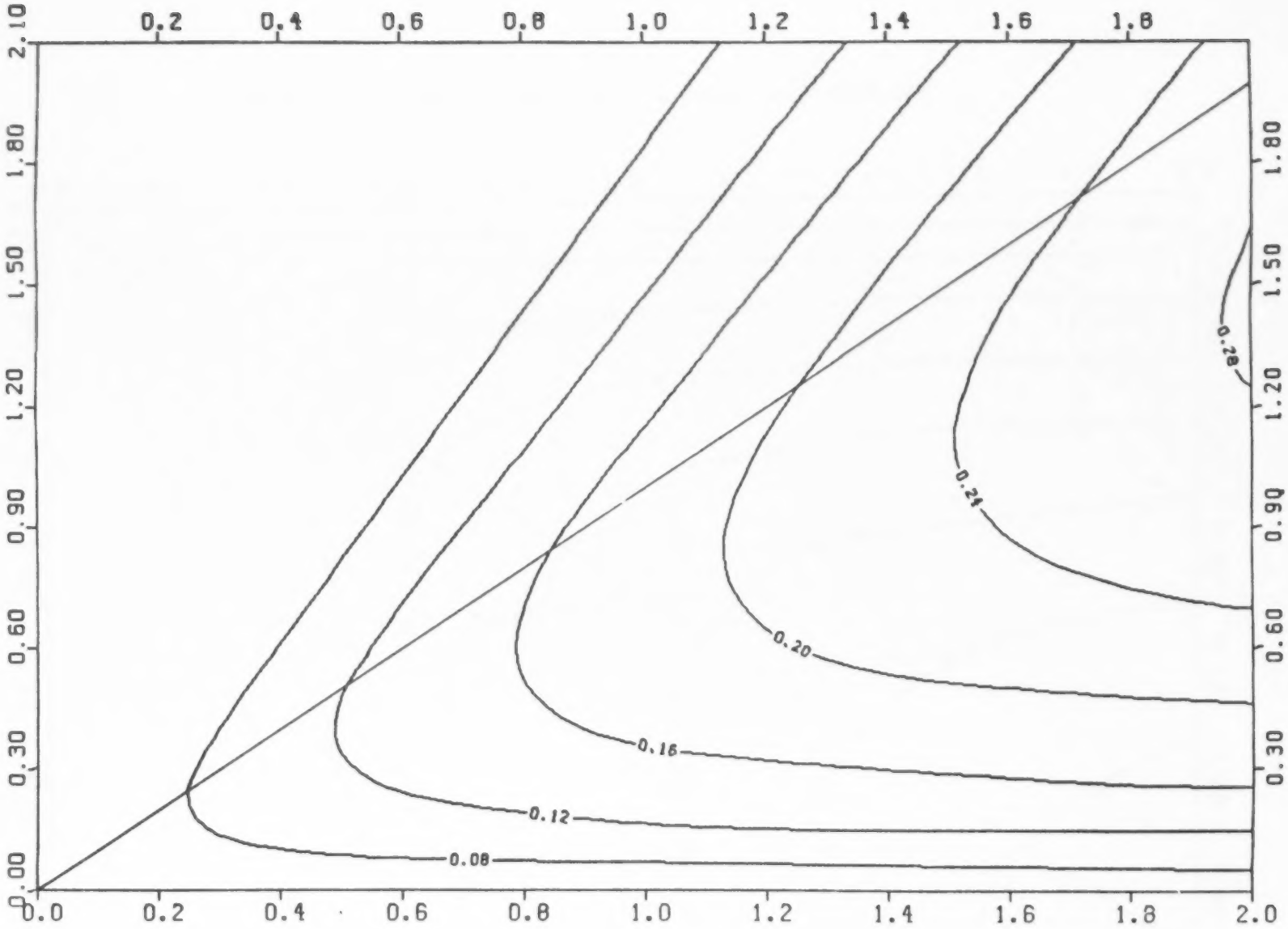


FIGURE IV-21. EKMA IIc TRAJECTORY: 26 JUNE 1982--DIFFERENT TRAJECTORY

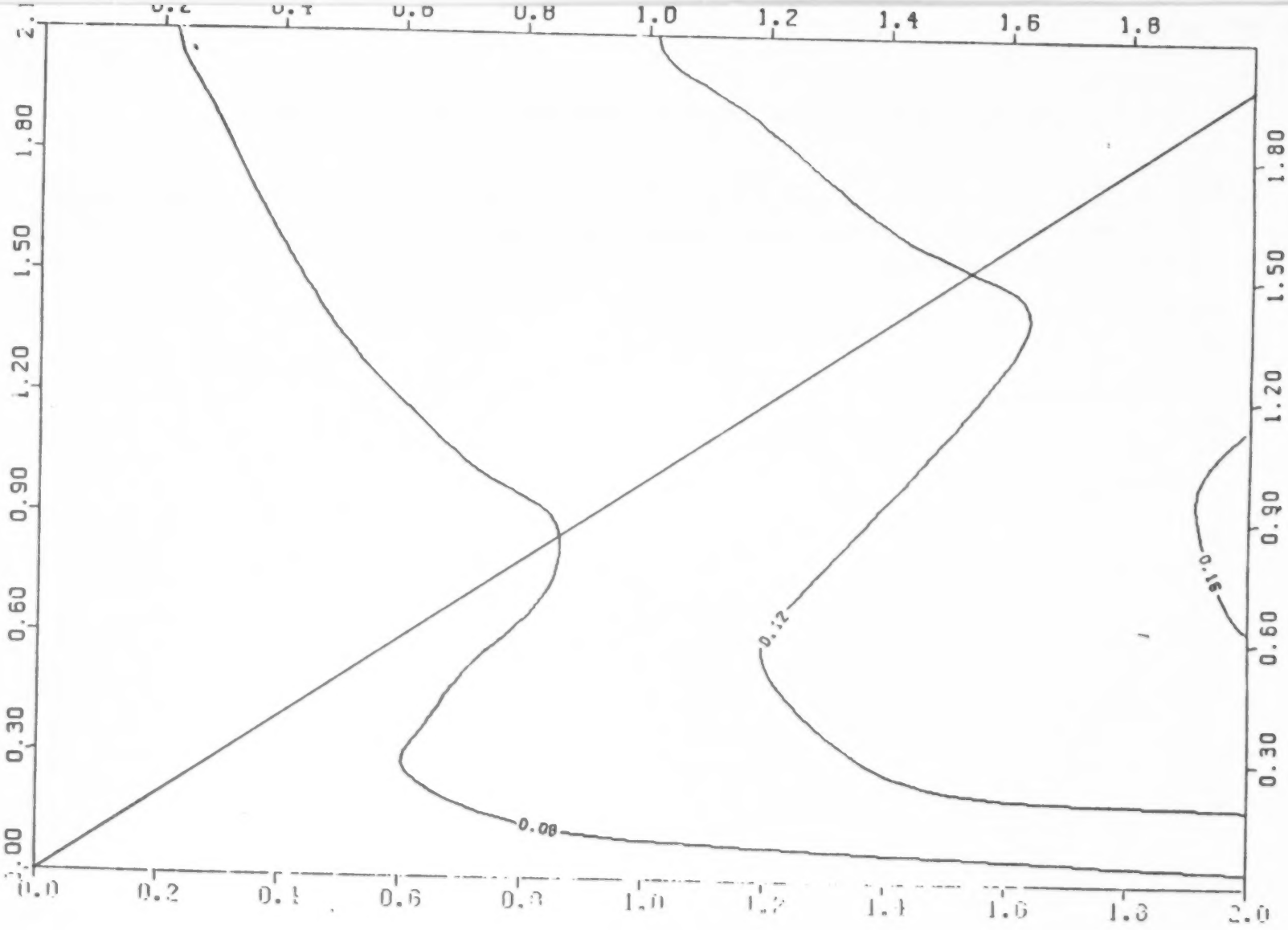


FIGURE IV-22. EKMA IIa TRAJECTORY: 27 JUNE 1982--DIFFERENT TRAJECTORY

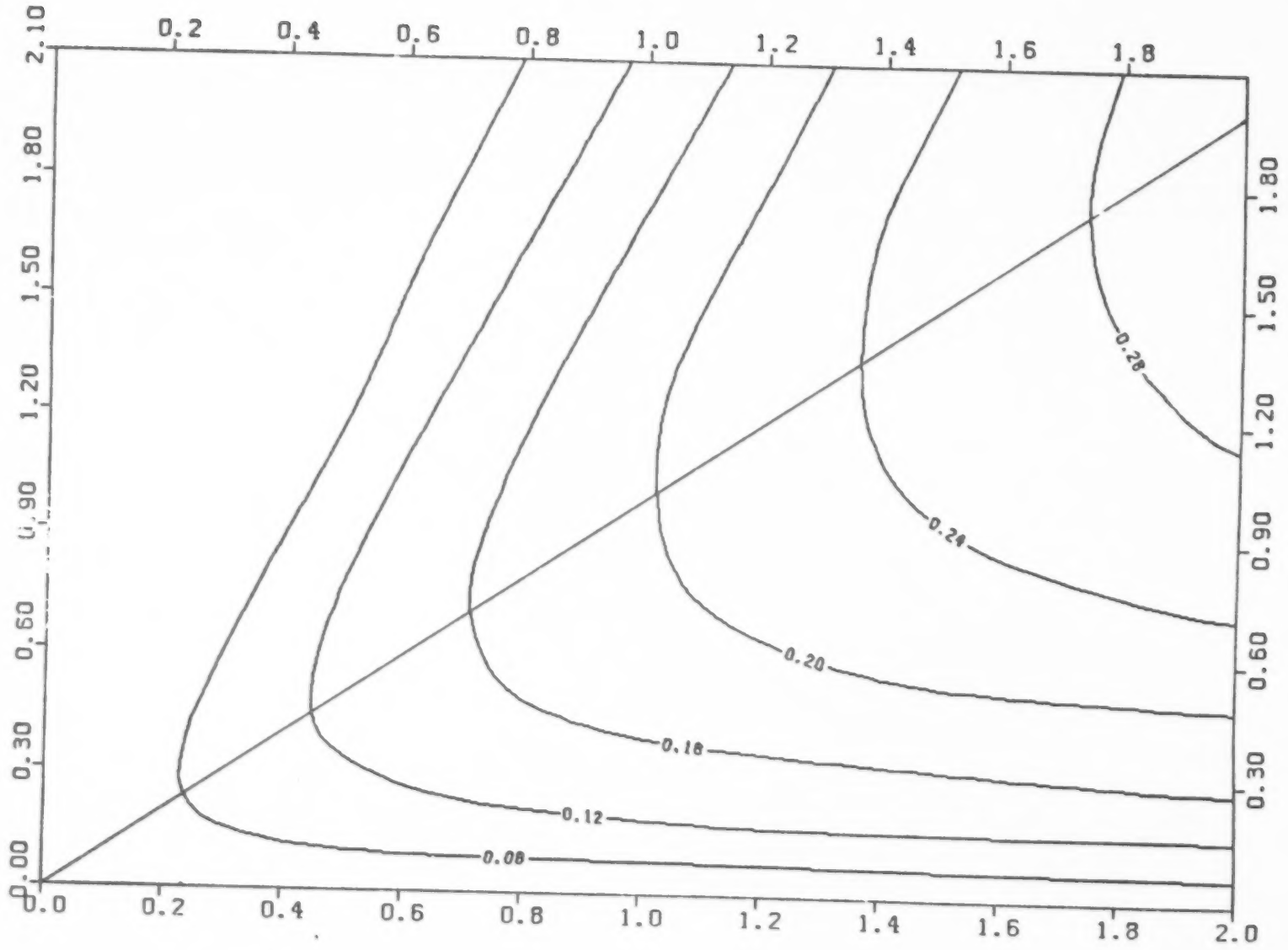


FIGURE IV-23. EKMA IIa TRAJECTORY: 4 AUGUST 1982--DIFFERENT TRAJECTORY

TABLE IV-5. OZONE PREDICTIONS FROM CBM-EKMA AND EKMA IIa MODELS

(a) Method (1):

> Total area emission changes
> Downtown Los Angeles 6:00 to 9:00 a.m. HC/NO_x from Airshed Model
> Design O_3 from Airshed Model

Date	CBM-EKMA	ΔO_3*	EKMA IIa	ΔO_3*
26 June 1974	0.12	-40	0.12	-40
27 June 1974	0.18	-44	0.19	-41
4 August 1975	0.14	-30	0.14	-30
26 June 1982	0.55	+90	0.53	+83
27 June 1982	0.60	+80	--	--
4 August 1982	0.33	+44	0.31	+35

(b) Method (2):

> Trajectory-specific emission changes
> Trajectory-specific 6:00 to 9:00 a.m. HC/NO_x
> Design O_3 from Airshed Model

Date	CBM-EKMA	ΔO_3*	EKMA IIa	ΔO_3*
26 June 1974	0.12	-40	0.11	-45
27 June 1974	0.15	-53	0.17	-47
4 August 1975	0.13	-35	0.13	-35
26 June 1982	0.54	+86	0.53	+83
17 June 1982	0.71	+122	--	--
4 August 1982	0.33	+43	0.31	+35

TABLE IV-5 (Concluded)

(c) Prediction Method:

> Total area emission changes
> Downtown Los Angeles 6:00 to 9:00 a.m. HC/NO_x from Airshed Model
> Observed design O_3

Date	CBM-EKMA	ΔO_3*	EKMA IIa	ΔO_3*
26 June 1974	0.18	-47	0.19	-44
27 June 1974	0.25	-49	0.26	-47
4 August 1975	0.21	-34	0.22	-31

* Percentage change in ozone = $\frac{(\text{Predicted } O_3) - (\text{Design } O_3)}{(\text{Design } O_3)} \times 100$

III-1, the value shown is 0.27 ppm for the CBM-EKMA compared with the 0.29 ppm value simulated by the SAI trajectory model, yet the isopleth result using the same trajectory predicts a value of 0.17 ppm. Investigation of the detailed computer outputs revealed that the primary explanation of this difference is found in the initial conditions used in the SAI trajectory model for 1982. These initial conditions were quite high in concentration for the first two 50-meter levels but the mixing height was initially only 50 meters. Hence, the rise in mixing height at 0600 (PST) brought in a significant amount of pollutants. In the original CBM-EKMA calculation this effect was simulated by a special addition to the emission vector at that hour (see table III-6).

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